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THE DEHYDROGENATION OF SEC-BUTANOL ON ALUMINA
CATALYST

BY



MAUNG NGE

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH
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OF MASTER OF SCIENCE IN CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL AND PETROLEUM ENGINEERING

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance a thesis entitled THE DEHYDROGENATION OF SEC-BUTANOL ON ALUMINA CATALYST submitted by MAUNG NGE in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

Date *May 5, 1972*

ABSTRACT

The vapour phase catalytic reactions of 2-butanol on sodium hydroxide treated alumina catalyst were investigated in a Pyrex flow reactor. A coupled Reactor-G.C. system was adopted and found to provide more accurate analysis than the conventional system.

The effects of temperature and contact time on the product distribution were determined at an average pressure of 700 mm Hg over the following range of operating conditions.

Temperature: 327°C to 414°C at a constant space velocity of
 2.468×10^{-2} mol/(hr)(gm of catalyst).

Space Velocity: 1.667×10^{-2} to 1.0173×10^{-1} mol/(hr)(gm of cat.)
at a constant temperature of 350°C.

Thermal decomposition of 2-butanol was not observed at temperatures below 447°C. The sodium hydroxide treated alumina catalyst catalyzed dehydrogenation of 2-butanol with very minor dehydration.

The rates of dehydrogenation at 350°C were obtained by analytically differentiating the function that was obtained by the least squares fitting of the kinetic data. A first order rate expression was found to fit the data well for the dehydrogenation of 2-butanol under the experimental conditions.

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CHAPTER 1

INTRODUCTION

The catalytic dehydrogenation of n-Propanol is very complex due to the number of side reactions taking place simultaneously. However, this is a reaction of both industrial and academic importance. Consequently many workers at the University of Alberta have studied this and related systems.

Hansen (1) used a fluidized bed to study the dehydrogenation of n-Propanol over an alumina supported chromia catalyst, but was unable to obtain reasonable yield of ketone. Vasudeva (2,3) suppressed the dehydrating tendency of a silica alumina catalyst by treating it with sodium hydroxide, thereby dehydrogenating n-Propanol to form diethyl ketone. Wanke (4) continued to study the kinetics of this system. Due to suspected thermal reaction and catalytic activity of stainless steel, Imai (5) worked on the thermal decomposition and the catalytic effects of stainless steel and Pyrex glass. Wanke (4) was unable to obtain sufficiently accurate kinetic data to permit kinetic analysis because of the complexity of the chemistry and the multiple chemical reaction steps involved (6). Therefore, Chan (7) using a simpler system investigated on the dehydrogenation of 3-pentanol, one of the intermediate products in the n-Propanol system.

With the ultimate aim of obtaining reliable kinetic data for the n-Propanol system, it was felt that an improved method of experimental technique would be necessary. A coupled reactor-gas chromatograph system was adopted for direct analysis of products. At the same time, collection of condensed liquid and gas products were separately done in order to compare the two methods of analysis.

It was considered that a simple kinetic study would be more suitable for the development of experimental technique. The dehydrogenation of sec-Butanol was chosen for the present investigation. Both sodium hydroxide treated silica-alumina and sodium hydroxide treated pure alumina catalysts were used.

The investigation also included measurement of kinetic data, improvement of product analysis and material balance and selection of the optimum experimental conditions to minimize side reactions.

CHAPTER 2

LITERATURE SURVEY

A literature survey was carried out in three areas, namely, experimental methods, chemical reaction and correlation of reaction rate data. In the section on experimental methods emphasis was placed on the importance of conducting experimentation in the region where mass and heat transfer would be negligible, because the object of a kinetic study is to determine the reaction on the catalyst surface. There was an abundance of literature on the dehydrogenation of 2-butanol, however, few workers reported using alumina as a catalyst. The third area covered the various methods of reaction rate data correlation.

2.1 EXPERIMENTAL METHODS IN CATALYTIC REACTIONS

Kinetics deals with the development of fundamental rate equations that fit the kinetic data and are consistent with observed reaction products. The attainment of a useful empirical rate equation is valuable in understanding and using a catalytic process (8).

Generally, kinetic measurements alone do not provide a complete picture of a catalytic reaction because it is concerned essentially with the slower steps of a reaction sequence. Other steps that influence the rate are the non-catalyzed processes such as diffusion, etc. Generally the process of finding kinetic equations for the catalytic reaction alone is difficult enough so that complications by mass and heat transfer should be avoided as much as possible.

However, reaction rate data obtained without evaluation of the diffusional effects can yield meaningless rate expressions that cannot be

applied directly in scale up for plant scale reactor design. Still in the design of reactors for commercial plants, reaction rate data from laboratory is often used. But considerable attention must be given to the non-chemical aspects of reactor behavior in scale up studies.

The object of investigations should be to determine the kinetics of the reaction at the surface without other complicating factors. Thus ideally the experimental laboratory catalyst bed should be (8):

- a) Isothermal.
- b) Inter- and intraparticle mass and heat transfer should be rapid compared with reaction rate.
- c) Plug flow or thoroughly stirred condition.
- d) Constant catalytic behavior over a substantial period of time.
- e) Accurate analytical methods for some or all of the components and products.

The designing of laboratory reactors is very well covered by J.J. Carberry (9) and other standard reaction kinetics references (10,11, 12,13).

2.2 CHEMICAL REACTION

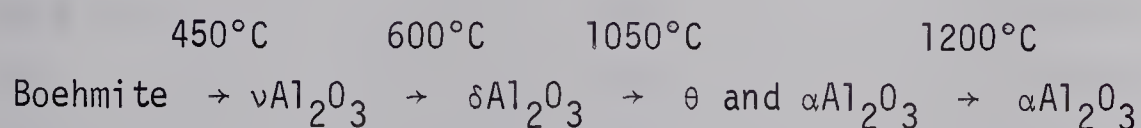
a) Decomposition of Alcohols

The catalytic decomposition of alcohols may proceed in two different directions, namely dehydrogenation and dehydration. The extent of each depends on the selectivity of the catalyst. By dehydrogenation the alcohol decomposes to form an aldehyde (for primary alcohols) or a ketone (for secondary alcohols) and hydrogen while on dehydration the alcohol gives an olefin and water. At high temperatures (300 - 600°C), severe decomposition of an alcohol may occur leading to the cleavage of carbon-

carbon bonds and the resultant formation of paraffins, CO, CO₂, etc. At near ambient temperatures, ether is the major reaction product.

b) Alumina as a Catalyst

Alumina is known to occur in several different crystalline structures by thermal decomposition of the hydrates, bayrite, or of the osyhydrate, boehmite. They can be represented by the following sequence (14):



The catalytic activity to a certain extent depends on which structure is present (4).

According to the well known principles of catalytic action, unstable species may result when a reactant molecule collides with the active centre of a catalyst. The nature and reactivity of these intermediates determine the products and the rate of reaction.

Catalysts may be classified according to different types of active centres (16) as follows:

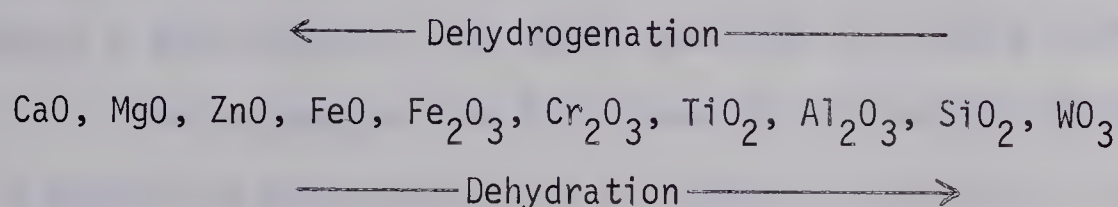
1. Oxidation - Reduction Catalyst (Roginskii's First Class).
2. Acid - Base Catalyst (Roginskii's Second Class).

Alumina is one of the typical acid solid catalysts of the second classification because of the presence of acid active centers at its surface (15). It is known to possess both Lewis and Bronsted acid centres. However, catalyst partition into the first and second class is not frequently as clear-cut as expected. Alumina functions as a first (dehydrogenation) or second (dehydration) class catalyst for the decomposition of ethyl alcohol. The extent of first and second class activity for

alumina and other oxides are shown below (16).

	$\begin{array}{c} \text{C}_2\text{H}_5\text{OH} \\ \text{at } 350^\circ\text{C \& 1 atm} \\ \swarrow \quad \searrow \\ \text{H}_2 + \text{C}_2\text{H}_4\text{O} \quad \text{H}_2\text{O} + \text{C}_2\text{H}_4 \end{array}$	
Oxide	First Class	Second Class
	%	%
Al_2O_3	1.5	98.5
Cr_2O_3	9	91
TiO_2	37	63
ZrO_2	55	45
Fe_2O_3	86	14
ZnO_2	95	5

Also, Batta (17) considers that the dehydrogenating activity of an oxide is a function of its ionic character and that as the covalent character of the oxide increases, it becomes more dehydrating.



However, as can be seen Al_2O_3 is predominantly a dehydration catalyst. Its activity is attributed mainly to the Bronsted type acid centres (14). Therefore very few studies have been made using Al_2O_3 as a dehydrogenation catalyst for alcohol decomposition.

Vasudeva (2) investigated the reaction of n-Propanol on sodium hydroxide treated alumina catalyst and found that the base-exchanged alumina becomes a dehydrogenating catalyst. Hagg and Pines (15) pointed

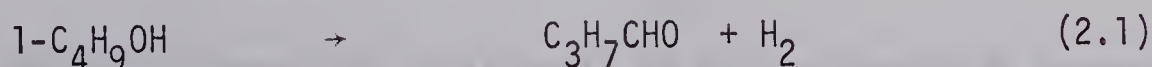
out that sodium treated aluminas exhibit catalytic properties towards hydrocarbons, similar to organosodium compounds in a homogeneous liquid phase. This sodium treatment can be pictured as a complete removal of protons from surface hydroxides and suppression of Bronsted acidity. This was verified by Dalla Lana (18) and Chuang (14) that only the Bronsted-acid sites (and not Lewis acid sites) react with the sodium hydroxide to form $=Al-O-Na$, and that a five to eight percent content of sodium hydroxide would totally suppress the dehydrating activity of Al_2O_3 to become purely a dehydrogenation catalyst, although a decline in catalytic activity per unit surface area was observed.

c) Chemical Reaction

The catalytic dehydrogenation of primary alcohols to aldehydes and secondary alcohols to ketones are well known chemical reactions. It was first studied by Ipatieff (19) who used such catalysts as a platinum tube, zinc rods, and brass for reaction with methyl, ethyl, isopropyl, isobutyl and isoamyl alcohols. Vasudeva (3) and Wanke (4) present a good review of the dehydrogenation of primary alcohols.

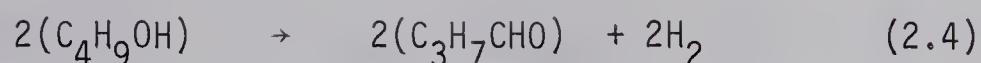
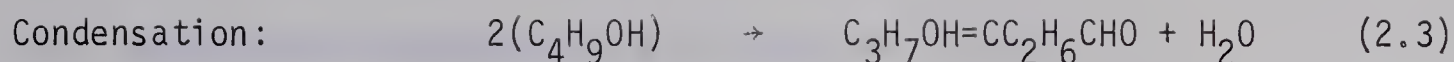
As an example, Rao (20) recently studied the dehydrogenation of 1-butanol to butyraldehyde on a catalyst containing 90% copper, 8% chromia and 2% carbon.

The reaction was mainly:



In addition, the following reactions are also possible:



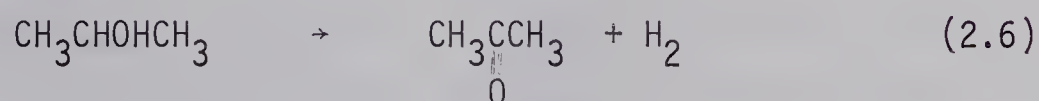


Tischenko's Reaction:

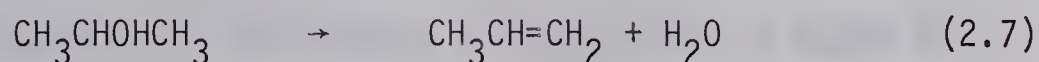


The dehydrogenation of sec-alcohols to ketones is more easily accomplished than primary alcohols since the ketones formed are more stable than aldehydes (4).

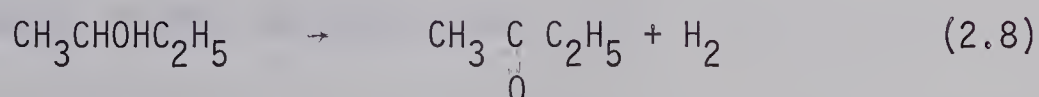
Because of the industrial importance, the dehydrogenation of isopropyl alcohol has been studied by many workers (14,21-26). The reaction is as follows:



Minor dehydration, according to the following reaction, was also reported

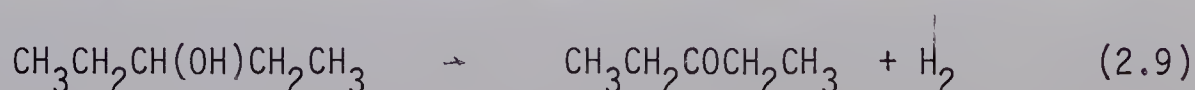


Dehydrogenation of sec-butyl alcohol to produce methyl ethyl ketone has also been studied by many workers (27,28,29,14).

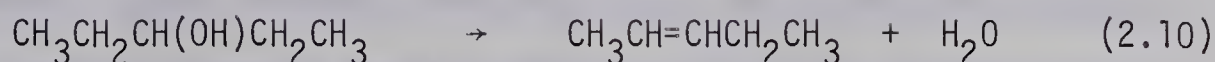


However, most of these studies were made over metals and metal oxide catalysts.

Very few dehydrogenation of alcohols on sodium hydroxide treated alumina catalyst has been studied (3,4,7,14). On secondary alcohols Chan (7) and Chuang (14) studied the dehydrogenation of 3-pentanol.



Small dehydration products were also found as follows:



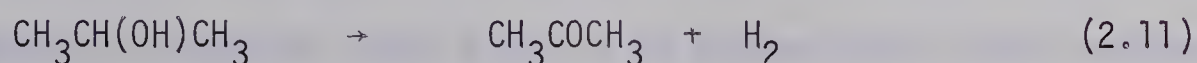
d) Thermal Decomposition

Perona (28) reported that less than 1% of sec-butanol feed into the glass reactor at 750°F without a catalyst emits an effluent gas with the following composition.

	Mole Fraction
Hydrogen	0.959
Methane	0.033
Ethane	0.001
Ethylene	<u>0.007</u>
	1.000

He indicated that the reaction is basically of a cracking nature.

Rice (30) reported on the thermal decomposition of lower aliphatic alcohols as mainly,



The ketone formed undergo further decomposition.



Imai (5) reported that the conversion of homogeneous thermal reaction of n-Propanol was 0.865 mol% at a temperature of 463°C. It was believed that the thermal decomposition can be avoided by studying the reactions at lower temperatures (below 450°C) in a glass reactor.

2.3 CORRELATION OF REACTION RATE DATA

Several types of models have been used for correlating reaction rate data. The most commonly applied model is the power function rate equation, for which the reaction order is selected by an analysis of experimental data. This method shall be referred to as the empirical approach.

It has become increasingly popular for chemical engineers to analyze the kinetic data for complicated solid-catalyzed gas reactions in terms of the extended Langmuir-Hinshelwood theory (31,32). This is generally known as the mechanistic approach.

2.3.1 Mechanistic Approach

Determination of the mechanism of a surface catalyzed reaction, or fitting a rate equation to data on such a system is accomplished by trial. Ordinarily, a large number of possible controlling steps must be investigated. This may be accomplished by some procedure like the following:

1. Various mechanisms are postulated. The Langmuir-Hinshelwood model supposes that the reaction takes place on an active site on the surface of the catalyst. The steps involved in the surface processes are:
 - a) Adsorption of a molecule on the active site.
 - b) The attached molecule then reacts either with another molecule on an adjacent site (dual-site mechanism) or with one coming from the main gas stream (single-site mechanism), or it simply decomposes while on the site (single-site mechanism).
 - c) Desorption of the product molecule from the surface to the fluid solid interface which gives the site further opportunity to adsorb

fresh reactants.

In the above three steps it is assumed that the transport of the reactants from the bulk phase to the solid catalyst surface and the transport of the products from the catalyst surface to the bulk fluid stream are not rate controlling.

2. Rate equations are written for each step. Several empirical constants occur in each such rate equation.

For example, the gas reaction, $A + B \rightarrow C$, is catalyzed by a solid. If it is assumed that a bimolecular surface reaction of A and B is rate controlling and that A, B, and C are adsorbed on the catalyst without dissociation, the reaction rate is written:

$$\text{Rate} = \frac{k p_A p_B}{(1 + K_A p_A + K_B p_B + K_C p_C)^2} \quad (2.13)$$

K_A , K_B and K_C are unknown adsorption coefficients characteristic of the individual gas. Other assumed mechanisms result in different equations.

3. The experimental data is now applied to evaluate the constants, which should all be either zero or positive. Any mechanism that yields one or more negative constants are to be rejected since the equilibrium and rate constants cannot be negative. The rate equation may be linearized. This permits the ready application of the method of least squares.
4. In any case in which there is more than one possible mechanism based on zero or positive constants, a choice between them can be made on the basis of goodness of fit to the experimental points.

The strongest argument in favour of this method is that if a mechanism is found which reasonably represents what truly occurs, extrapolation to new and more favorable operating conditions is much more safely done.

2.3.2 Empirical Approach

The conventional methods of determining the reaction order and estimating the rate constant can be broken down into four primary areas (12,33,34). These methods are generally used for homogeneous reaction systems but may also be applied to heterogeneous systems when surface reaction controls.

a) Method of Integration

In this method, a reaction order is assumed and the differential rate equation is then integrated to provide an equation relating an instantaneous concentration to the time over which the reaction has taken place. For example, a second-order equation might be written:

$$-\frac{dC_A}{dt} = kC_A^2 \quad (2.14)$$

so that upon integration:

$$\frac{1}{C_{A_0}(1-x)} - \frac{1}{C_{A_0}} = kt \quad (2.15)$$

Several techniques exist for testing this integrated equation and thus the assumed reaction order.

To test graphically the adequacy of the integrated equation one can plot the concentration function, such as $1/C_{A_0}(1-x)$, vs. time. If

the correct order has been chosen, in this example second order, the data can be well correlated by a straight line, the slope of which provides an estimate of the rate constant.

b) Method of Differentiation

It can be seen that if one can obtain the reaction rate itself, that is, the rate of change of concentration with time in Equation (2.14) in the previous method, the slope of the logarithm of the rate versus concentration will directly give the reaction order. The determination of this rate requires differentiation of the concentration-time data. Several methods of accomplishing this have been suggested (33,35). In one of these, the concentration-time data can be fitted by an empirical function which may be differentiated analytically to obtain reaction rates.

c) Method of Fractional Life Times

The most commonly used fractional life is the half-life, i.e. the time required for one half of a given reactant to be consumed (12, 33,34). For the half-life, an integration of, for example, Equation (2.14) yields

$$t_{1/2} = \frac{1}{k C_{A_0}} \quad (2.16)$$

Then the rate constant can be evaluated from measurements of the half-life for several initial concentrations noted to determine the adequacy of the assumed reaction order. This method is practical only on homogeneous reaction systems.

d) Method of Reference Curves

Walas (12) discusses a method of assessing the reaction order

without estimating the rate constant. Here, the ratio of the time required to reach any conversion divided by the time required to reach, say, 90% conversion is plotted against conversion. The data can be shown to be a function only of the reaction order, and can be plotted on a graph containing a group of reference curves for given orders. Thus, the experimental order can be obtained by matching the data to one of the curves.

The mechanics of applying these various techniques and the influence of experimental error on the reaction order estimated is very well discussed in the literature (12,33,34).

CHAPTER 3

EXPERIMENTAL APPARATUS

Figure 3-1 shows the overall layout of the equipment and instrumentation used to control the feed rates, the vaporizer and reactor temperatures.

3.1 ALCOHOL FEED SYSTEM

A syringe type micro-feeder was employed for the alcohol feed system. The sec-butanol was fed by a 100 cc leakproof brass syringe with teflon o-ring seals and a uniform diameter piston. The piston was driven for precise and stable feed rate by a synchronous motor through a system of gears, manufactured by Azuma Denki Kogyo Co. Ltd., Tokyo, Japan. Different feed rates were obtained by changing the combination of transmission gears. Five different syringe piston velocities were used in this investigation. The calibration is given in Appendix I.

3.2 INERT NITROGEN FEED SYSTEM

Nitrogen feed to the preheater was controlled at a constant pressure of 30 psig by means of the nitrogen cylinder regulator and a Nullmatic pressure regulator. The flow rate was regulated by a Nupro stainless steel bellows valve and was measured by a Matheson mass flow meter, Model 1f-20. The mass flowmeter consists of an electrically heated tube and an arrangement of thermocouples to measure the differential cooling caused by a gas passing through the tube. The thermoelectric elements generate a dc voltage proportional to the rate of mass flow of gas through the tube. There are no fragile sensing elements projecting into the stream. This design depends only on the mass flow

and specific heat of the particular gas and is therefore almost insensitive to pressure and temperature changes. The calibration of the mass flow meter is given in Appendix II.

3.3 VAPORIZATION SYSTEM

The vaporizer was fabricated from a one meter length of 1/16 inch O.D. type 316 stainless steel tubing turned into spirals of 3 cm diameter, and placed in an oil bath, dimensions 12 cm diameter by 30 cm high. The oil used was primal 855 oil obtained from Imperial Oil Limited, and was heated by a 1000 watt calrod heater positioned as a helical coil on the inside wall of the vessel. A schematic cross-section of this system showing the location of the vaporizer in the oil bath is shown in Figure 3-1. The container was surrounded by 5 cm thickness of asbestos insulation. The bath was also equipped with a stirrer, driven by a three speed electric motor. The oil temperature was measured by a ceramic insulated metal sheathed 1/16 inch O.D. iron-constantan thermocouple, purchased from Thermo Electric Company (Catalog No. 5J0411e). The oil temperature was controlled by a Honeywell R7161J Versatronik SCR Trigger Controller with Digital Setpoint. Good temperature control was obtained with this apparatus and the bath temperature did not fluctuate more than 1°C when sec-butanol was fed at the feed rates employed. The oil bath was lifted and lowered by a pneumatic lift which simplified handling.

The nitrogen gas was preheated in the same oil bath. The gas was passed into the vaporizer through a 250 cm length of 1/4 inch stainless steel tubing, turned into spirals of 8 cm diameter, the latter part of which also served as the outlet line for the vaporized sec-butanol.

A 12/5 female metal ball-socket joint was attached to the end of this line for connection with the reactor inlet.

3.4 REACTION SYSTEM

The reactor was made of Pyrex glass. The inlet of the reactor was jointed to the outlet of the vaporizer by a 12/5 male glass ball socket joint. After this joint, the reactant and product flow lines were all made of Pyrex. The upper dead volumes within the reactor above the inlet and the outlet were decreased by placing the Pyrex tubes inside the reactor (5). The thermocouples were located inside these tubes to prevent the reactant and products from contacting the stainless steel of the thermocouple. Three thermocouples were used to measure the inlet, the reactor bed and the outlet temperatures.

The reactor was heated by a eutectic salt bath, with dimensions of 13.5 cm inside diameter by 35 cm high. The composition was 50 wt percent sodium nitrate and 50 wt percent potassium nitrate. The salt was heated by a 2500 watt calrod heater placed as a helical coil on the inside wall of the vessel containing the salt and the reactor.

A schematic cross-section of this system is as shown in Figure 3-1. The container was surrounded by 5 cm of asbestos insulation. The bath was also equipped with a stirrer driven by a three speed electric motor. As before, the bath was raised and lowered by a pneumatic lift.

The temperature in the salt bath was controlled by a Foxboro Model 64100 FO temperature recorder-controller. A Foxboro type 693 EMF converter equipped with a 1/4 inch iron-constantan thermocouple supplied the input to the controller which regulated the current to the calrod

heater. Excellent temperature control was obtained in this way and the bath temperature did not fluctuate more than 0.5°C once a steady temperature in the bath was obtained. The temperature range over which the controller will regulate the temperature depends on the range unit in the emf converter. A $300\text{--}500^{\circ}\text{C}$ range unit was used for the present program.

The thermocouples used for measuring the temperature inside the reactor were ceramic-insulated, metal sheathed $1/16$ inch O.D. iron constantan thermocouple, purchased from Thermo Electric Company (Catalogue No. 5J0411e).

The pressure difference between the system and the atmospheric pressure was measured by a monometer placed after the reactor outlet as shown in Figure 3-1. The pressure difference was found to be negligible.

3.5 SAMPLING SYSTEM

The sampling system was divided into two sections:

a) Direct Sampling and Analysis

In the direct (or coupled) sampling/analysis, the product stream from the reactor was carried through a $1/4$ inch Pyrex glass line into the sample valve of the gas chromatograph. The glass line was heated by Nikrothal wire wrapped around the whole length whose outside surface was covered by $1/2$ cm thickness of asbestos insulation. The temperature of this line was controlled by varying the input voltage of a powerstat power supply, as shown in Figure 3-1. A shielded $1/16$ inch O.D. iron constantan thermocouple was installed just before the inlet to the sample valve so as to measure the temperature of the incoming stream into the gas chromatograph.

b) Indirect Sampling and Analysis

To prevent condensation of the vapour products in the line between the reactor exit and the condenser, Nikrothal wire was wrapped around this line with asbestos tapes over it. The Nikrothal wire was heated by the same powerstat power supply described above. During start-up and shut-down, the products were vented through the direct line. At a steady-state defined by constant temperature and feed rate, the products were passed through an ice-cooled water condenser and then into a cold trap which was immersed in an ice-water mixture.

The non-condensable gases passed from the cold trap to a 75 cc gas sampling tube and then into the wet test meter. The wet test meter used was of Precision make with a 0.1 cu. ft. capacity per revolution. The accuracy of the wet test meter used was checked and found to be within $\pm 2\%$ of the actual gas flow.

3.6 TEMPERATURE RECORDING

The two thermocouples from the reactor were connected to a Speedomax Type G Leeds and Northrup 12 point variable range variable zero temperature recorder. The time required to complete the 12 point cycle was 48 seconds. The thermocouple on the line from the vaporizer to the reactor system was also connected to this recorder. A thermocouple was placed to measure the temperature of the products just before entering the sample valve in the gas chromatograph and it was also connected to the recorder. The range, normally set on this recorder, was checked and adjusted prior to every experimental run by feeding voltage into the recorder from a potentiometer, equivalent to those produced by an iron constantan thermocouple at 100°C and at 350°C. The same was

done for the runs made above 350°C. An ice water cold junction was used for all thermocouples other than the one attached to the temperature controller since the controller was equipped with a cold junction compensator.

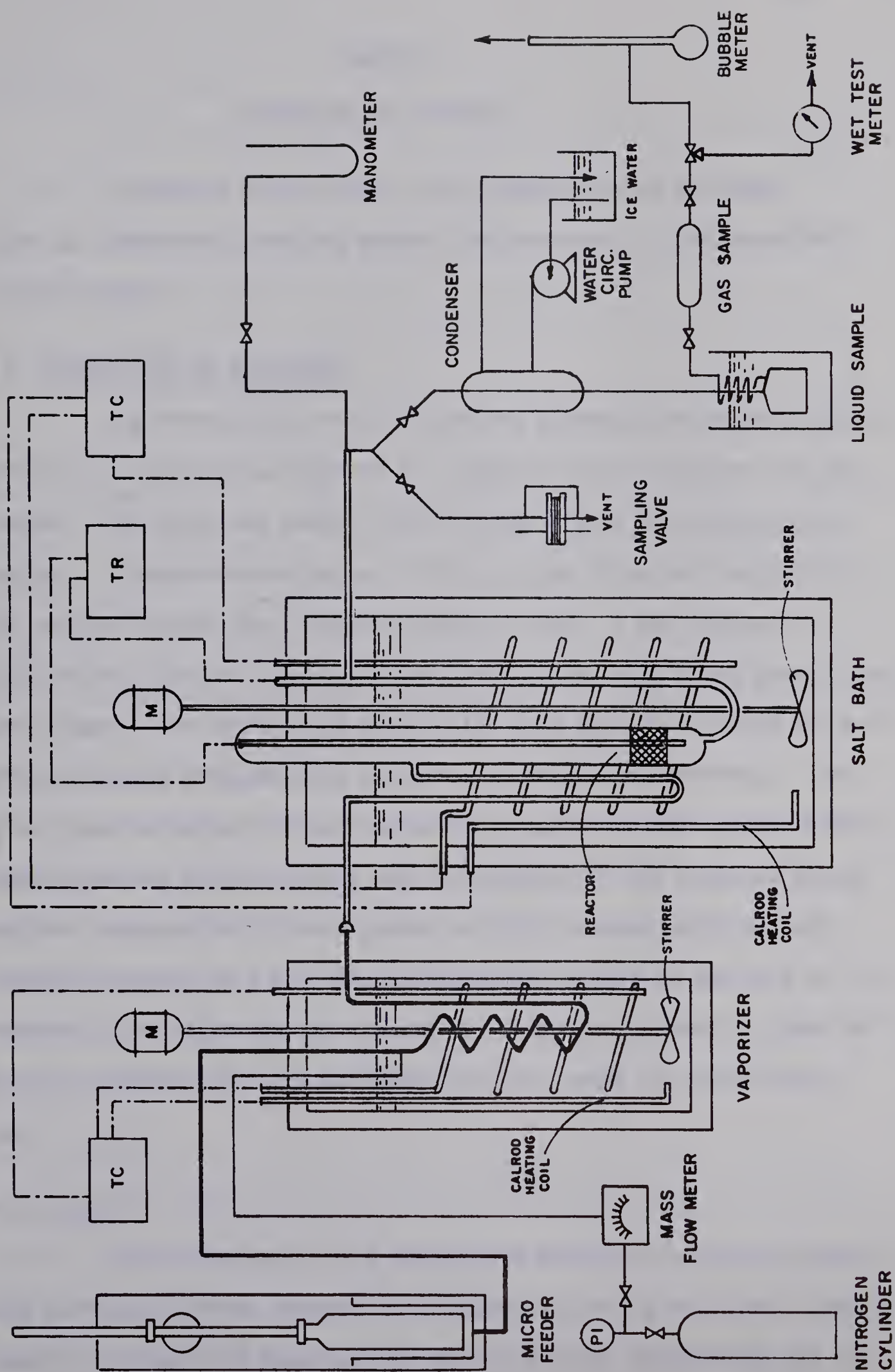


FIG. 3-1 SCHEMATIC LAYOUT OF EQUIPMENT

CHAPTER 4

OPERATION OF EQUIPMENT

A detailed description of the preparation of equipment, start-up, operation, sampling phases, and shut-down of the operation is given below.

4.1 PREPARATION OF EQUIPMENT

The Pyrex glass container for the thermocouple to the catalyst bed and the porous glass support for catalyst were introduced into the reactor. The joint was sealed with silicone grease and secured with springs. A predetermined amount of Pyrex glass chips was charged into the reactor through the catalyst charging inlet. A new charge of catalyst was then put in, and on the top of this, more Pyrex glass chips were placed. The inert Pyrex glass chips were used to minimize the end effects arising from the flow pattern and temperature gradients. The Pyrex glass container for the thermocouple measuring the reactor outlet temperature was put into place and the opening for the catalyst charge was then sealed with silicone grease and again secured with springs. The whole reactor unit was then fastened and secured to the rest of the equipment with clips and the connections wrapped with heating tapes to prevent condensation. The equipment was then ready for experimental runs.

4.2 START UP

The calrod heater and temperature controller of the oil bath were switched on after immersing the vaporizer in the oil bath. Approximately 90 minutes of heating time was required to achieve the set

temperature of 166°C.

The reactor was immersed in the salt bath after the salt was completely melted at about 300°C. A proportional band setting of 15% with a 4.5 minute reset was then used on the automatic temperature controller to give a minimum of cycling or over-shooting. Steady bath temperature was achieved after approximately three hours. The lines at the exit of the vaporizer and the reactor were then heated to about 140°C and 125°C, respectively, by adjusting the input voltage of the powerstat power supply. The whole system was then purged with nitrogen. The sampling valves were switched to direct sampling system after the nitrogen gas had passed through the sample collecting system for about 15 minutes. Once steady state temperatures and set nitrogen gas flow rate conditions were obtained, the apparatus was ready for experimentation.

4.3 STEADY STATE OPERATION

When a new charge of catalyst was used, steady state conditioning for a certain period of time was required to stabilize the activity of the catalyst. This was done firstly by establishing the desired feed rate of sec-butanol and secondly by analyzing the non-condensable gas products every 15 minutes until two similar chromatograms were obtained (approximately one hour).

4.4 SAMPLING

The columns used in the gas chromatograph during the direct sampling and analysis runs will be described later. A sampling valve in the gas chromatograph was used to inject the vapour products into the column system. A sampling loop of 5 cc by volume was installed in the

system. The flow of products during sampling is as shown in Figure 4-1. Before sample injection, the product stream flows through the sampling loop, position (a) in the figure. At sample injection, a pneumatically operated slider placed the sample loop in the carrier gas line, and the sample was swept into the column, position (b) in Figure 4-1.

Thus a chromatogram was obtained by switching the sample valve once steady state was obtained.

After injection, the vapour products obtained were discarded by venting through a cold trap. At the same time, preparation was done for collecting the sample for indirect sampling and analysis. The ice-water cold trap was installed and ice-cooled water was circulated through the condenser. The sampling was started by diverting the product flow to the other branch of the sampling system by switching the two valves simultaneously and the time was recorded by a stop watch. The sampling time was 30 minutes. After the sampling period, the product flow was vented by switching the two valves simultaneously again.

The liquid product obtained was sealed with stoppers and weighed immediately. A noncondensable gas sample was collected in a 75 cc gas sample tube. The total gas flow was read from the wet test meter.

4.5 SHUT DOWN

The alcohol feeder, heaters, stirrers, ice water circulation pump, recorders and controllers were shut off in this sequence. Flow of nitrogen gas into the system was maintained for about 15 minutes to purge the equipment. The oil bath and salt bath vessels were lowered with the pneumatic lifts. The salt bath was lowered while the salt was

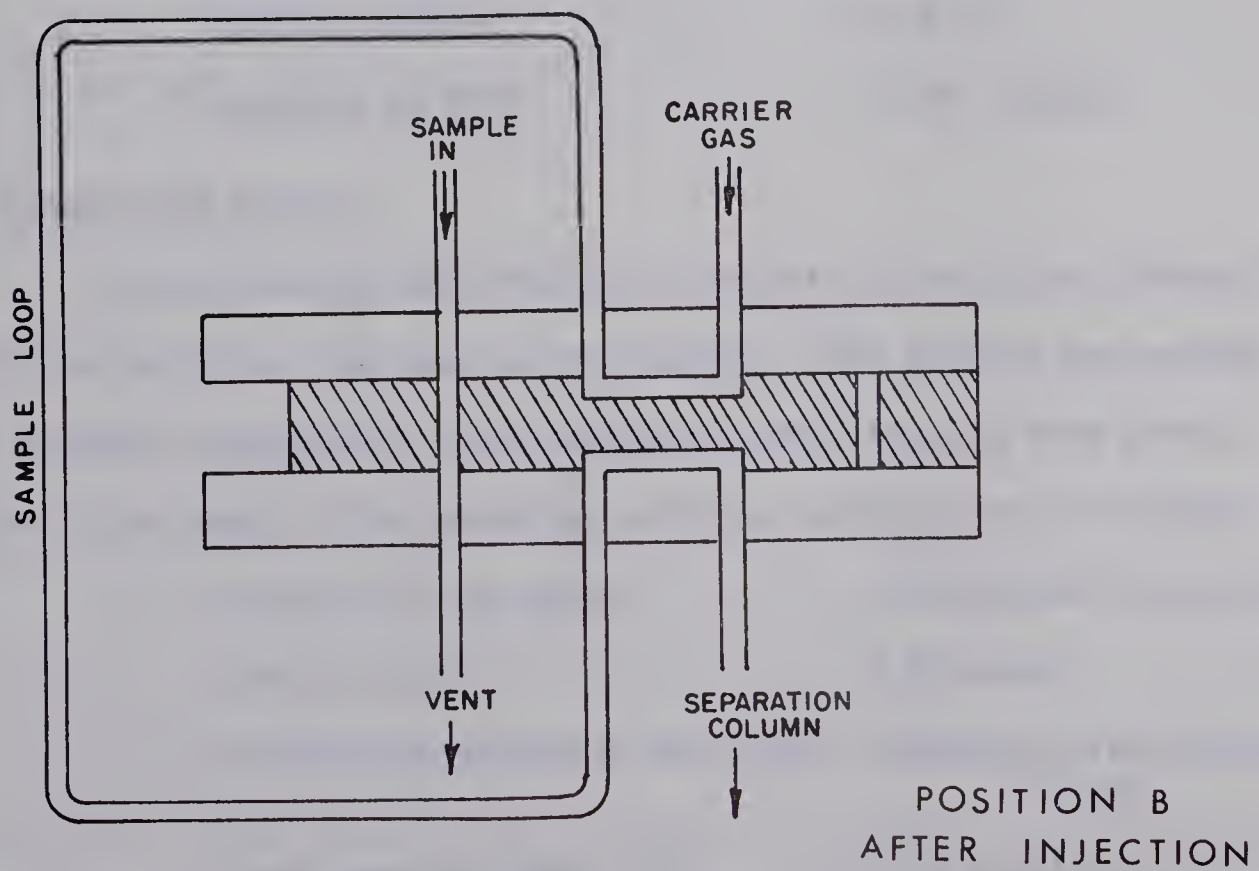
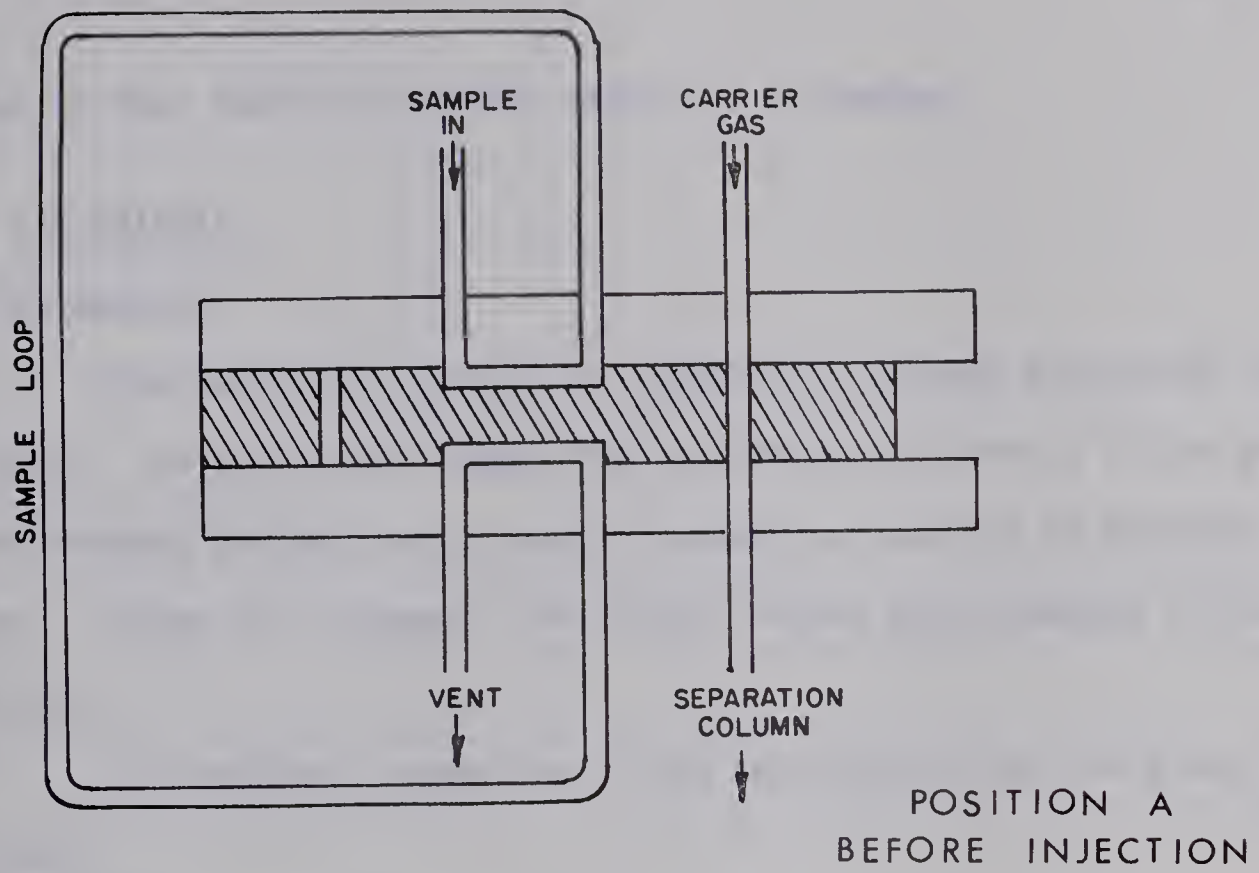


FIG. 4-1 SAMPLING VALVE

molten so that the glass reactor might not be damaged.

4.6 RAW MATERIAL

a) Sec-Butanol

The sec-butyl alcohol was supplied by Eastman Industries (Cat. No. 943). The purity was higher than 99.97% by peak area % of gas phase chromatography analysis using Ucon Chromosorb column (to be described later). Traces of 1-propanol and diethyl ketone were detected in the analysis.

The physical properties of the sec-butanol (36) are given as follows:

Molecular Weight	74.12
Specific Gravity	0.808 20/4
Boiling Point	99.5°C
Density at 20°C	6.74 lbs/gal

b) Pyrex Glass Packing

Pyrex packing was obtained by crushing Pyrex glass tubing, the quality of which is the same as the reactor. The packing was washed with acetone, aqueous HCl, NaOH solutions and water and then dried before it was used. The properties of Pyrex packing are as follows:

Particle Size Range	-10 +20 mesh fraction
Density (37)	2.23 gm/cc
Thermal conductivity @25°C(37)	0.0023 cal/(sec)(sq.cm) (°C/cm)
Mean specific heat (37) 25°C - 175°C	0.20 cal/(gm)(°C)

Composition (37)

Silica	80%
Boric oxide	14%
Soda	4%
Alumina	2%

c) Alundum Catalyst

The physical and chemical properties are given in Table 4-1. The 1/8" x 1/8" cylinders of alundum were crushed and the -10 +20 mesh fraction was immersed in 2N sodium hydroxide solution for 6 hours. The excess solution was filtered off and the solids were dried at 150°C for 5 hours.

d) Pure Alumina Catalyst

The physical and chemical properties are given in Table 4-2. The catalyst was treated with 2N NaOH by the same procedure as above.

4.7 PRODUCT ANALYSIS

All product samples were analyzed by using a Beckman Model GC4 Gas-Liquid Chromatograph, using a thermal conductivity detector. The peak areas of each chromatogram were integrated by using an Aerograph Model 471 Digital Integrator manufactured by Infotronics Corporation.

Extensive work was done on GC separation and column development. Liquid phases that were reported to provide good separation for alcohols, ketones, aldehydes (38) were tested. The following were the columns prepared and tested besides the ones that were used in the present work:

1. 25 feet of 1/8 inch diameter copper tubing packed with Apiezon M on Chromosorb W (-80 +100 mesh).

TABLE 4-1

PROPERTIES OF ALUNDUM CATALYST

Manufacturer: Norton Company of Canada, Ltd.

Manufacturer's Designation: LA-617

Properties as specified by manufacturer:

1. Chemical (Typical) Analysis:

Al_2O_3	=	77.0%	K_2O	=	0.2%
SiO_2	=	21.2%	MgO	=	0.2%
* Fe_2O_3	=	0.2%	CaO	=	0.2%
Ti_2O	=	0.5%	ZrO_2	=	-
Na_2O	=	0.5%			

*Note: All elements are reported as metal oxides. The actual presence of the metals is in the form of complex silicates and/or aluminates.

2. Physical Properties:

Porosity	=	60-65%
Water absorption	=	51-56%
Bulk density	=	1.1-1.2 gm/cc
App. Sp. Gr.	=	3.0-3.2 gm/cc
Packing density	=	46 lbs/cu.ft.
Surface area	=	60-70 sq meters/gm
** after treated with NaOH	=	26 sq meters/gm
Max. service temp.	=	700°C
X-Ray analysis	=	predominantly γ -alumina some α -alumina and quartz

**Note: Measured by Sorptomat.

TABLE 4-2

PROPERTIES OF PURE ALUMINA CATALYST

Manufacturer: Houdry Process and Chemical Company

Manufacturer's Designation: HA-100S

Properties as specified by manufacturer:

1. Chemical (Typical) Properties:

Al_2O_3	wt %	98.5
Na_2O	wt %	0.1-0.2

2. Physical Properties

Surface Area	m^2/g	75-85
Bulk Density	kg/l	0.78-0.82
Pellet Density	kg/l	1.28-1.34
True Density	kg/l	3.6-3.7
Porosity	Vol. %	60-65
Crushing strength	lbs	15-30
Knife-edge Hardness	1000 g	5-10

2. 25 ft of 1/8 inch diameter copper tubing packed with Porapak R (-100 +120 mesh).
3. 12 ft of 1/8 inch diameter copper tubing packed with squalane on Chromosorb W (-80 +100 mesh).
4. 25 ft of 1/8 inch diameter copper tubing packed with 30% Ucon on acid washed chromosorb W (-80 +100 mesh).

The length and diameter of the columns were in accordance with reference (39) using liquid samples collected by the conventional system (indirect sampling), extensive tailing with bad resolution results except for column 4. However, when column 4 was used on the direct sampling/analysis system, resolution was poor because the vapour sample injection was not sharp as in the liquid samples. This resulted in the preparation of a longer column (40 ft) for the present investigation.

Four columns were required to effect a complete separation of the components in the samples. The following is a description of the type of column used and the operating conditions under which the product analysis was carried out.

- a) Column: This column was made from 40 ft of 1/8 inch diameter copper tubing packed with 30% Ucon in acid washed Chromosorb W (-80 +100 mesh). The Ucon Lubricant LB-1800x, was supplied by the Union Carbide Chemical Company.

Column Temperature: 120°C for coupled system.

150°C for conventional system of liquid product.

(Difference due to different sample injection system).

Detector Temperature: 200°C

Detector Current: 200 mA

Sample Size: Coupled system vapour product @ 140°C: 5 cc

Conventional system liquid product @ 21°C: 0.5 microliter

Carrier & Reference Gas: Helium

Gas Flow Rate: Carrier side: 25 cc/min

Reference side: 25 cc/min

Components Separated: Nitrogen, butene-1, trans-butene-2, cis-butene-2, methyl ethyl ketone, 1-propanol, sec-butanol, diethyl ketone.

- b) Column: 1/8 inch diameter, 6 feet long stainless steel tubing packed with Porapak S (-100 +120 mesh).

Column Temperature: 140°C

Detector Temperature: 200°C

Detector Current: 200 mA

Sample Size: 0.5 microliter

Carrier & Reference Gas: Helium

Gas Flow Rate: Carrier 30 cc/min

Reference 30 cc/min

Components Separated: This column was mainly used for the analysis of water. The components separated under the above conditions were air, water, butenes, methyl ethyl ketone, and sec-butyl alcohol.

- c) Column: 30% Ucon on acid washed Chromosorb W (same as Column (a)).

Column Temperature: 35°C

Detector Temperature: 100°C

Detector Current: 200 mA

Carrier and Reference Gas: Helium

Gas Flow Rate: Carrier 30 cc/min

Reference 30 cc/min

Components separated: Nitrogen, butene-1, trans-butene-2, cis-butene-2.

- d) Column: 1/8 inch diameter, 25 ft. long, copper tubing packed with activated charcoal, supplied by Burrell Corporation (Catalogue No. 341-10).

Column Temperature: 60°C

Detector Temperature: 100°C

Detector Current: 200 mA

Carrier & Reference Gas: Helium

Gas Flow Rate: Carrier 30 cc/min

Reference 30 cc/min

Components Separated: Hydrogen, nitrogen and methane.

The products were identified by their respective retention times obtained by passing pure samples of both liquid and gases involved through the appropriate columns. They were further confirmed by mass spectrometer analysis.

4.8 CALIBRATION OF APPARATUS

Calibration of the Matheson Mass Flow Meter for the Nitrogen feed stream, the microfeeder for the sec-butyl alcohol feed, the thermocouples were done prior to the start of the experimental program.

Calibration procedures are presented in Appendices I and II.

CHAPTER 5

EXPERIMENTAL PROGRAM AND RESULTS

The present investigation was carried out at approximately 700 mm Hg. and at temperatures from 330°C to 420°C with the following objectives.

1. To investigate the thermal decomposition of sec-butyl alcohol.
2. To compare activity of NaOH treated Alundum and NaOH treated pure alumina catalyst.
3. To measure the life of the catalyst.
4. To find the effect of temperature on product distribution.
5. To find the effect of film diffusion.
6. To find the effect of pore diffusion.
7. To find the effect of space velocity on product distribution.

The approach taken, the experiments done and the results obtained are outlined in detail in the following section.

5.1 DEFINITION OF TERMS

Terms used in reporting the results are defined below.

a) Reaction Temperature

The reaction temperatures reported were those recorded by the thermocouple located at the centre of the catalyst bed. These temperatures corresponded approximately to the mean of the temperatures measured at the top and the bottom of the catalyst bed.

b) Space Velocity

Space velocity is defined for the present work as:

$$\text{Space Velocity} = \frac{\text{moles of sec-butanol feed}}{(\text{hr.})(\text{gm. of catalyst})}$$

c) Conversion

$$\text{Conv. of sec-BuOH} = \frac{\text{moles of sec-butanol converted}}{\text{moles of sec-butanol in feed}}$$

$$\text{Conv. by Dehydrogenation} = \frac{\text{moles of MEK formed}}{\text{moles of sec-butanol fed}}$$

$$\text{Conv. by Dehydration} = \frac{\text{moles of butenes formed}}{\text{moles of sec-butanol fed}}$$

d) Material Balance

Material Balance provides a measure of the accuracy of the experimental data.

For coupled system:

$$\text{Overall Material Balance (\%)} = \frac{\text{Sum of Wt. of components in product}}{\text{Wt. of sec-butanol in feed}} \times 100$$

For conventional system:

$$\text{Overall Material Balance (\%)} = \frac{\text{Wt. of Gas product} + \text{Wt. of Liquid product}}{\text{Wt. of N}_2 \text{ fed} + \text{Wt. of sec-butanol fed}} \times 100$$

e) Carbon, Hydrogen and Oxygen Balance

These gram atom balances are used as a measure of the completeness and reliability of product analysis.

$$\text{Carbon Balance} = \frac{\text{gm. atoms of carbon in analyzed product}}{\text{gm. atoms of carbon in sec-butanol fed}} \times 100$$

Similar definitions apply to Hydrogen and Oxygen Balances.

5.2 THERMAL DECOMPOSITION OF SEC-BUTANOL

Four experimental runs were performed to investigate the effect of temperature and Pyrex surface on the thermal decomposition of sec-butanol. A slow feed rate of 6.2767 gm of sec-butanol per hour and 9.2600 gm Pyrex packing were used for all these runs. The reaction was studied at temperatures of 329, 398, 419, and 447°C. Temperatures above 447°C were not used because excessive side reactions would result. No inert nitrogen gas was fed into the reactor.

Analysis of the product revealed only sec-butanol and trace amount of impurities from sec-butanol feed, which indicates that Pyrex has no effect on sec-butanol and furthermore that homogeneous thermal decomposition did not occur under the experimental conditions.

5.3 ACTIVITY OF NaOH TREATED ALUNDUM AND PURE ALUMINA CATALYST

A set of 8 runs, runs 1 to 8, was carried out with NaOH treated Alundum catalyst at constant space velocity and various temperatures. The experimental results are shown in Appendix V and Figure 5-1.

Another set of 14 runs, runs 10 to 23, was carried out with NaOH treated pure alumina catalyst at same constant space velocity and various temperatures. The experimental results are again shown in Appendix V and Figure 5-1.

It is noted that the conversion of NaOH treated pure alumina is higher at all temperatures than that of NaOH treated Alundum catalyst, and that the difference in conversion is highest at about 350°C. Therefore it was decided to carry out the subsequent experimental runs with NaOH treated alumina catalyst.

5.4 EFFECT OF TEMPERATURE ON PRODUCT DISTRIBUTION

Runs 10 to 23 were also done to study the effect of temperature on product distribution. The experimental results are shown in Appendix V and Figure 5-2.

It is noted that at 350°C the reaction consists of dehydrogenation and dehydration at sec-butanol conversion of 0.16, the extent of side reaction being negligible. Therefore it was decided that subsequent experimental runs be carried out at 350°C.

5.5 EFFECT OF TIME ON CATALYTIC ACTIVITY

Runs 10, 16, 19, 22 and 23 were carried out to study the effect of time on catalytic activity at constant temperature of 367°C and a constant feed rate of 0.16925 gm mol sec-butanol per hour. Appendix V and Figure 5-3 show the results obtained in terms of 2-butanol conversion. The catalytic activity remained fairly constant between 3 to 34 hours of use. Thus samples were taken after about three hours of operation when the system reached steady state. There were no experimental runs with any batch of catalyst that was carried out beyond 30 hours of operation. Therefore it can be said that the following experimental runs were performed within the period of constant catalyst activity.

5.6 EFFECT OF SPACE VELOCITY ON PRODUCT DISTRIBUTION

Two sets of experimental runs, runs 24 to 36, were carried out to investigate the effect of space velocity on product distribution at a constant temperature of 350°C. Two charges of catalyst 3.3845 gm and 5.0774 gm were used. The result of these runs are shown in Appendix V and Figure 5-4. The reaction pressure of all runs was constant at 700 mm Hg.

5.7 EFFECT OF FILM DIFFUSION

The interpretation of experiments become difficult when more than one resistance affects the rate. To avoid this problem, it is important to first find the limits of operation where the various resistance must be considered.

Experimental runs 24 to 36 were also designed to study the effect of film diffusion. Some of the conditions of the experimental runs were such that the space velocity was constant but at varying flow rates of identical feed. Where film diffusion does not influence the reaction rate, conversion should remain the same at all feed rates. The results are shown in Appendix V and Figure 5-5.

5.8 EFFECT OF PORE DIFFUSION

Since catalytic reactions take place at surfaces through processes of adsorption and desorption, any alteration of surface area will naturally cause a change in reaction rate. Therefore catalyst area is an important variable which has to be considered.

Catalyst studies are frequently carried out on plane surfaces, such as platinum, mercury etc. and the measured reaction rates are usually expressed as per unit area of the catalyst. However this study as in most industrial catalyst, is carried out on porous material (alumina), which results in a much larger amount of active area per unit volume of reactor. Since the effective internal area of the catalyst pellet is quite unknown, it is more convenient to express the reaction rate as being unit mass of the catalyst. The rate now is obviously dependent on the porosity of the pellet.

Before catalysis can take place, the reagents have to diffuse through the pores and it can occur that either reaction or diffusion is the rate controlling process or that both of these have an almost equal effect.

It follows that the size of the catalyst pellet may or may not have an influence on the reaction rate per unit mass. If diffusion is so effective that the internal surface is fully used, the pellet dimensions will have little influence since the external area is usually small compared to the internal area. However if pore diffusion is the significant factor it would be an advantage to reduce the pellet size. That is, conversion will be higher with smaller catalyst size.

To investigate this, experimental runs 24 and 37 were made using charges of catalyst of equal weight but different particle sizes under same operating conditions. The results are shown in Appendix V and Table 5-1.

TABLE 5-1
EFFECT OF PORE DIFFUSION

Run No.	24	37
Reaction Temp. ($^{\circ}\text{C}$)	347.6	348
Wt. of Catalyst (gm.)	3.3845	3.3848
Space Velocity (mol./hr.g.)	.05000	.05000
Particle Size (mesh)	-10+14	-14+20
2-Butanol Conversion	.131	.132
Material Balance (%)	98.75	96.45

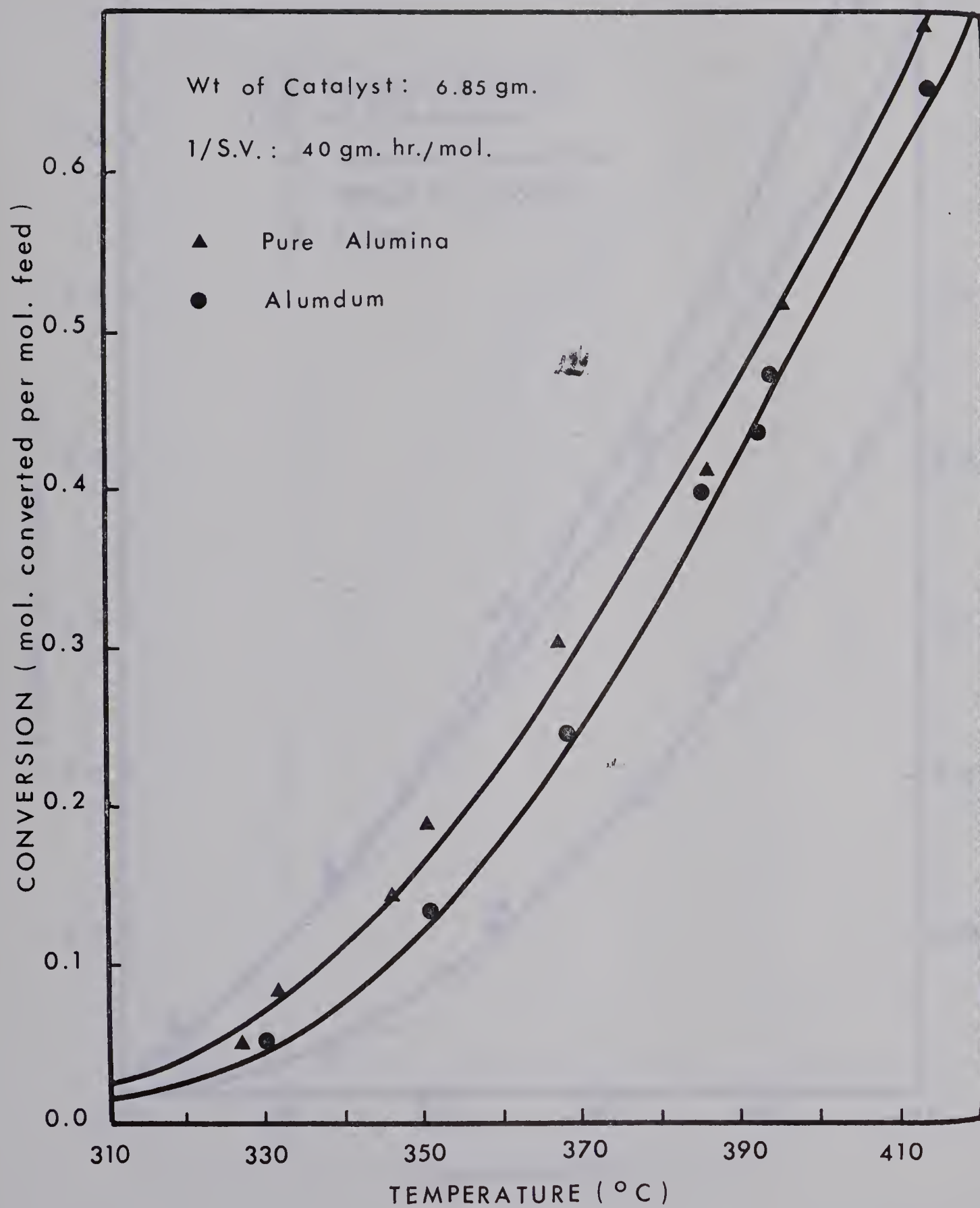


FIGURE 5-1. COMPARISON OF CATALYTIC ACTIVITY

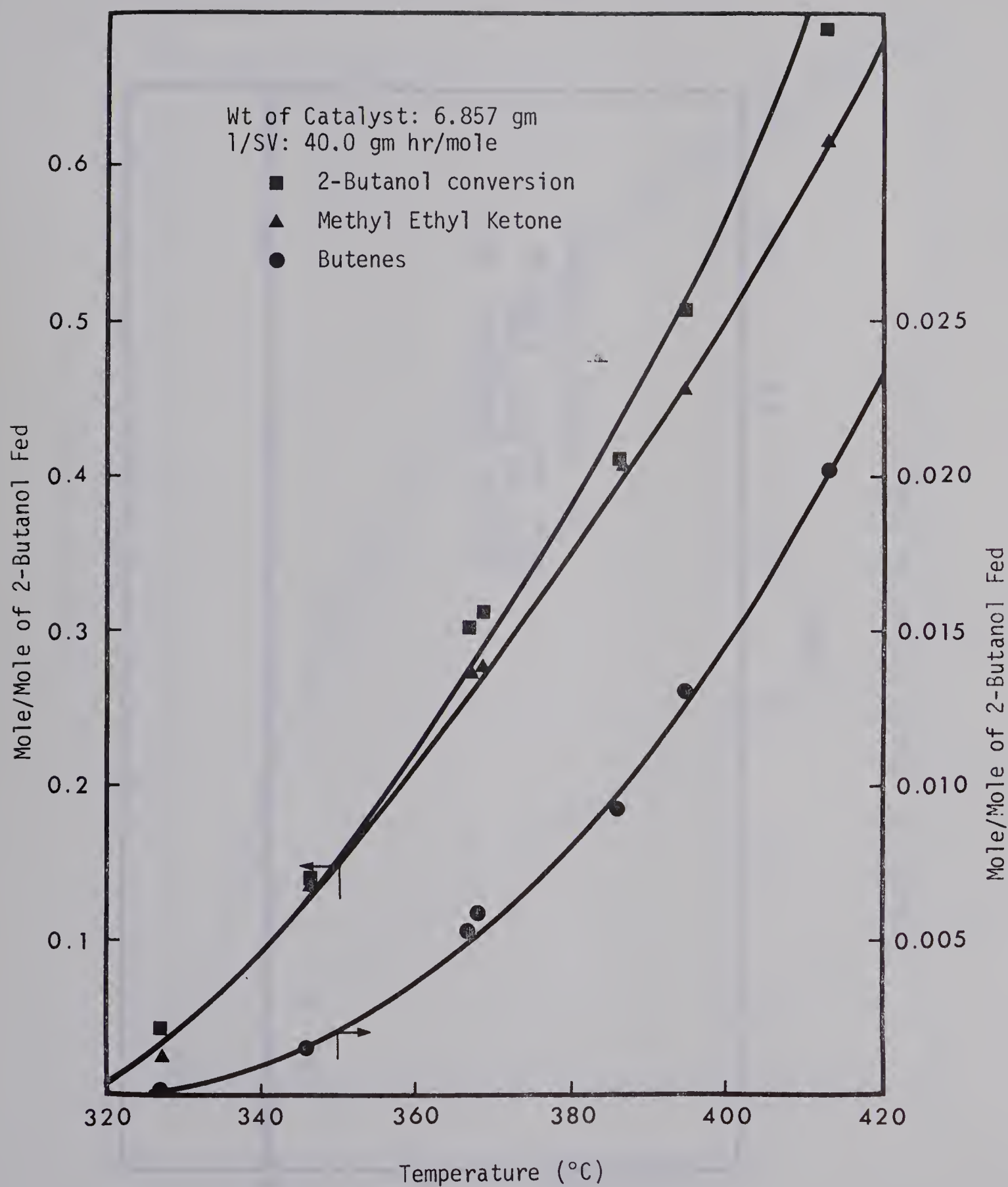


FIGURE 5-2. EFFECT OF TEMPERATURE ON PRODUCT DISTRIBUTION

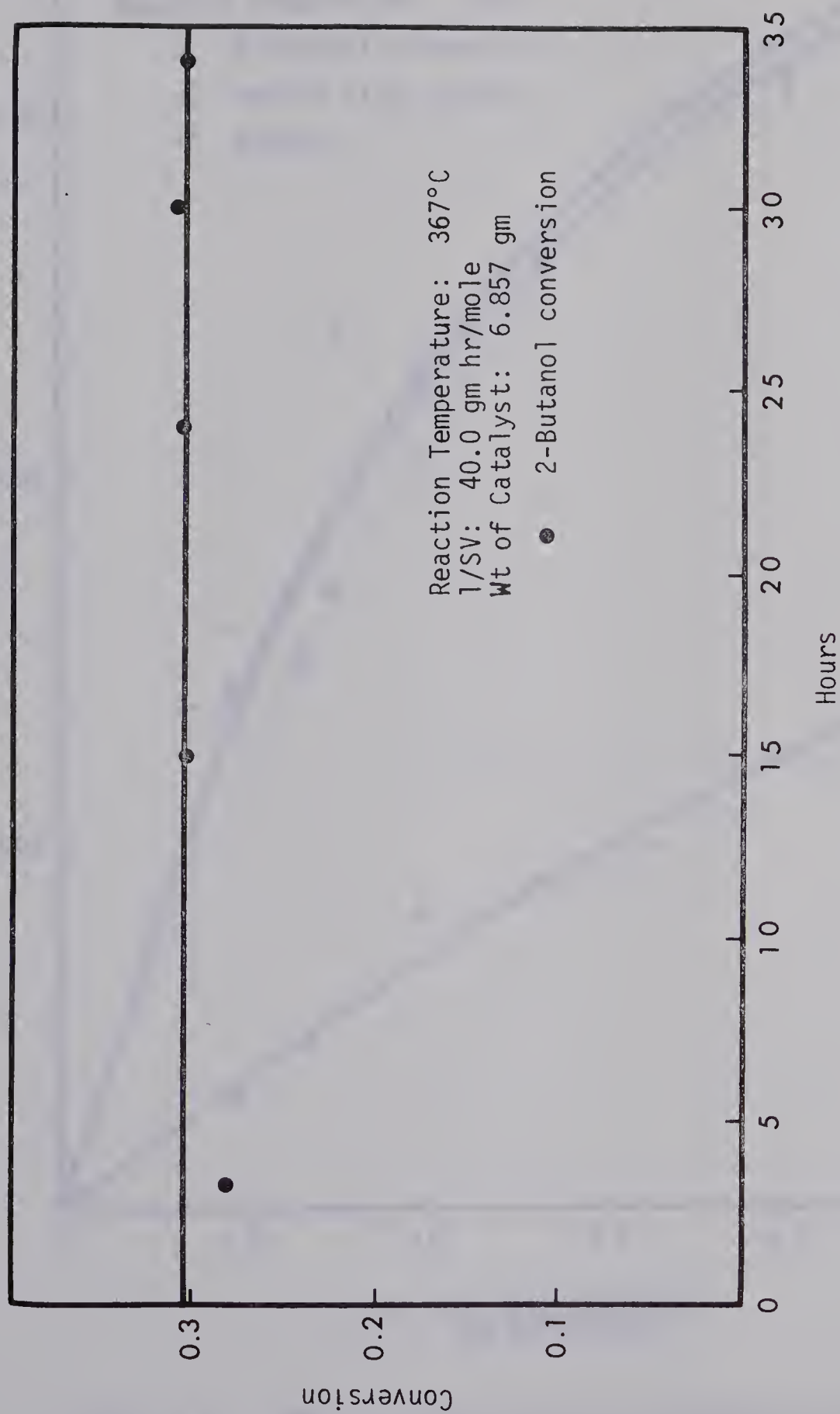


FIGURE 5-3. EFFECT OF TIME ON CATALYTIC ACTIVITY

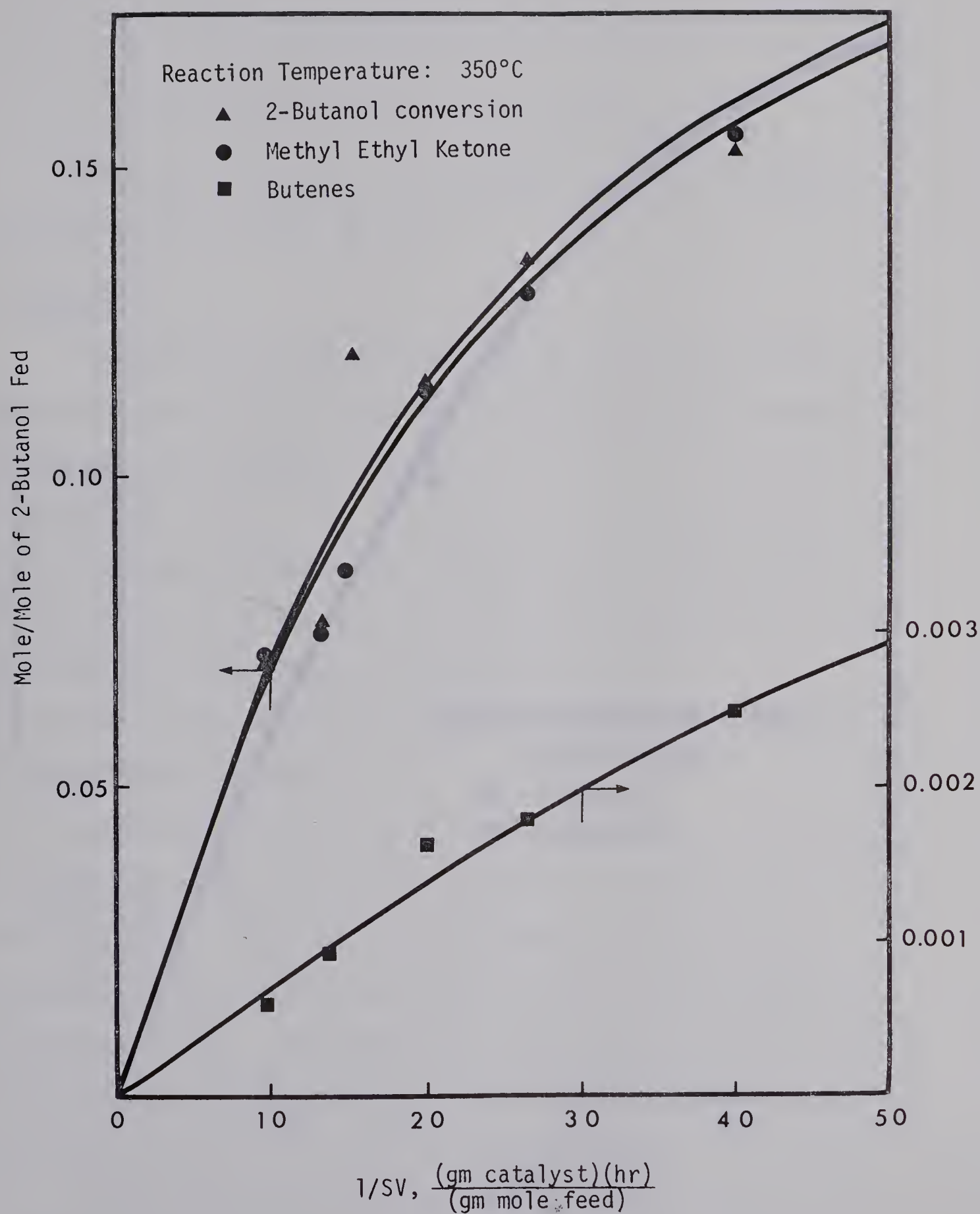


FIGURE 5-4. EFFECT OF SPACE VELOCITY ON PRODUCT DISTRIBUTION

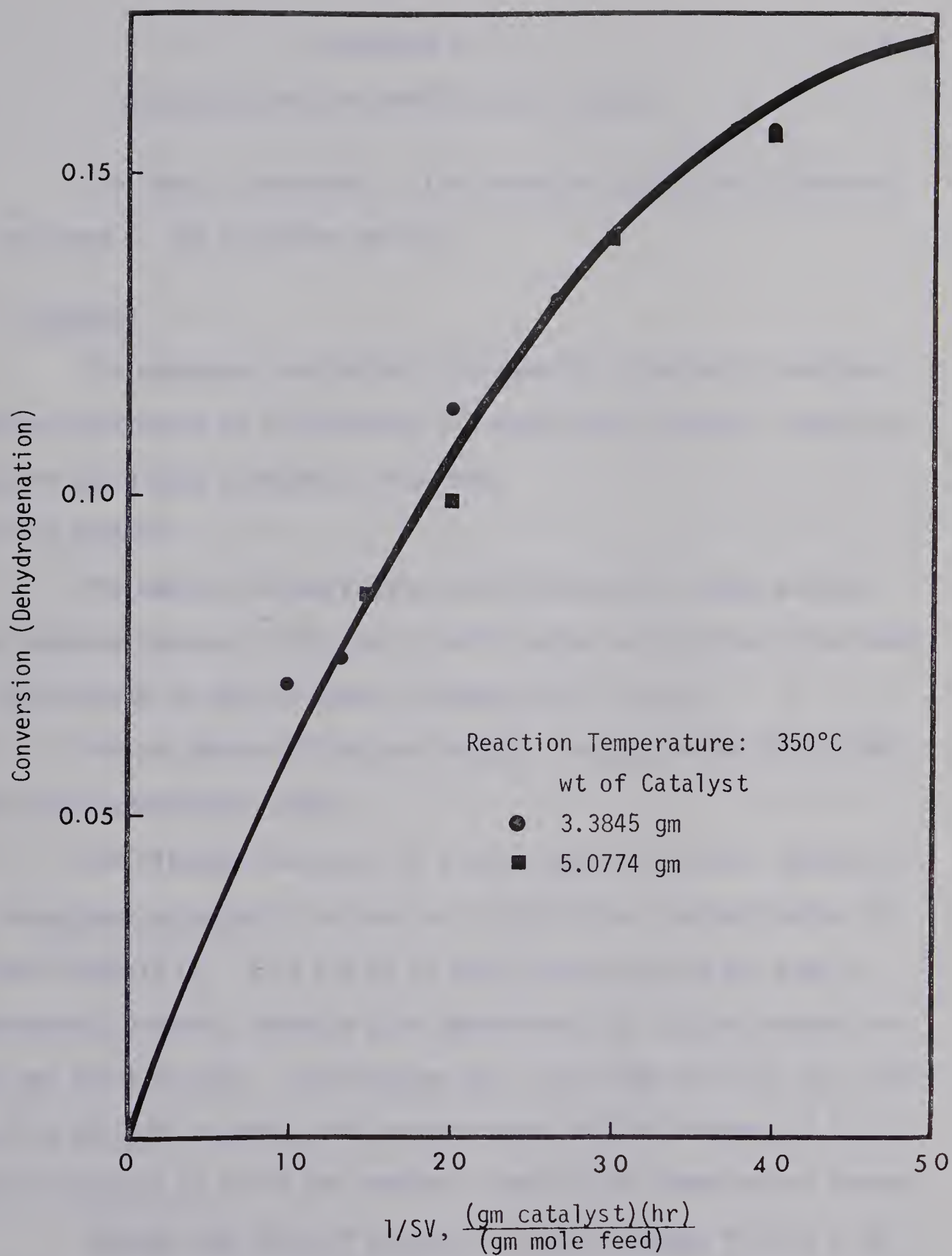


FIGURE 5-5. EFFECT OF FILM DIFFUSION

CHAPTER 6

DISCUSSION AND INTERPRETATION OF RESULTS

The results presented in the preceding section are discussed and analyzed in the following section.

6.1 EQUIPMENT

The equipment can be best discussed by dividing it into two sections consisting of flow control and temperature control. Reaction pressure was always constant at 700 mmHg.

a) Flow Control

The control of sec-butanol and nitrogen flow rates was more than adequate because of the use of micro feeder and the mass flow meter. The calibration of them is shown in Appendices I and II.

The sec-butanol flow rate produce a maximum error of $\pm 0.24\%$ within the experimental range.

The nitrogen feed rate is a very important factor, because of the dependence of material balance on it during the Coupled Reactor GC System (Appendix IV). This had to be done because during the time of experimental program, accurate flow measurement for the hot vapour product was not available. The Matheson Mass Flow meter used for the nitrogen flow had good accuracy with maximum error of 0.4% between 15 to 20 cc/min (Appendix II) which was generally used in the experimental program.

However the ratio of alcohol to inert nitrogen feed is a far more important factor and should be as small as possible. This ratio was about 2 to 9 in this experimental program. This was not small enough a ratio because a 1% error in the mass flow meter would be magnified 3 to

10 times in the material balance. However it was used because the mass flow meter has a maximum range of 20 cc/min. Therefore for the maximum error of 0.4% on the flow meter, the error of the material balance can be said to be about a maximum of 4.0(0.4x10%). This will be discussed in more detail later.

b) Temperature Control

The temperature controller of the oil bath in the vaporization system was very good. Bath temperature did not fluctuate more than $\pm 1^{\circ}\text{C}$.

The temperature control for the reactor was done by controlling the salt bath temperature. The Foxboro temperature controller was excellent and the bath temperature did not fluctuate more than $\pm .5^{\circ}\text{C}$ once a steady temperature in the bath was obtained. The thermocouple measuring the reaction temperature indicated a temperature below the actual bath temperature (3°C) because of the heat transferred from the reactor wall through the catalyst bed and finally through the glass thermocouple container.

6.2 PRODUCT ANALYSIS

The analysis of the product samples and the use of the relative response factors to calculate mole percent of each component was quite accurate as indicated by the test samples and the material balance and carbon, hydrogen, and oxygen balances of each sample. The balances are given in Appendix V.

To check the accuracy of the relative response factors as described by Messner (40), six standard samples were prepared with various concentrations of sec-butanol, methyl ethyl ketone and benzene and were weighed using an analytical balance. The purity of the components were

checked by the gas chromatography, and were all found to be over 99% purity. Benzene was added to the mixture as a reference. The peak areas were then obtained from the gas chromatograph of the mixture and the relative response factors of the components were calculated by using the following equation:

$$f_i = \frac{\text{wt. percent}_i \times \text{Area benzene}}{\text{wt. percent benzene} \times \text{Area}_i}$$

wt. percent_i = wt. percent of component i in the calibration mixture.

Area_i = peak area of i measured directly from chromatogram.

A complete calculation of the prepared samples is shown in Appendix VI. The relative response factors obtained by this calculation compared very closely with those given by Kaiser (41) as shown in Appendix VI. Therefore the relative response factors given by Kaiser can be considered to be reliable and were used for this work. The relative response factor for hydrogen was taken from Anderson (42).

6.3 COUPLED REACTOR-GAS CHROMATOGRAPH SYSTEM

In the conventional system of product analysis, the vapour products leaving the reactor are usually condensed by passing through a condenser and collected in some type of cold trap (for the present work, the cold trap was immersed in an ice-water mixture). The condensed liquid product sample is then weighed and analyzed. The noncondensable gas products are usually measured (a wet test meter was used for the present work) and collected in some gas sampler and analyzed separately. By this method, product loss can occur during the sampling processes and this shows up in the material balance.

To prevent this product loss, the Coupled Reactor-GC System was adopted, where the hot vapour product was introduced directly into the gas chromatograph for analysis without condensation. However, as mentioned in Section 6.1, the accuracy of the coupled system is very dependent on the accuracy of the inert nitrogen flow rate and the ratio of alcohol to nitrogen feed rate. The material balances of the experimental runs for both the coupled system and the conventional system are shown in Appendix V and compared in Table 6-1.

Although the ratio of alcohol to nitrogen used was not optimum (because of the limit on the maximum range of N_2 flow meter), it can be observed that the material balance for the coupled system was generally better than that for the conventional system. The same can be said for carbon, hydrogen and oxygen balances in Table 6-1. The superiority of the coupled system will be further verified in Section 6.9.

TABLE 6-1
COMPARISON OF MATERIAL BALANCE FOR CONVENTIONAL AND COUPLED SYSTEM

Run No	Material Balance		Carbon Balance		Hydrogen Balance		Oxygen Balance	
	Conventional System	Coupled System	Conventional System	Coupled System	Conventional System	Coupled System	Conventional System	Coupled System
1	95.57	96.73	96.39	96.26	96.91	97.14	97.74	97.88
2	98.16	97.48	98.44	97.24	98.24	97.11	99.51	98.42
3	101.41	99.91	97.08	99.67	98.30	96.90	97.90	102.49
4	96.15	96.64	96.88	96.04	97.28	97.70	98.13	97.78
5	97.85	95.23	97.77	94.97	98.15	95.56	98.16	95.82
6	99.14	97.16	98.66	96.78	98.83	96.96	100.28	98.44
7	97.44	98.35	98.00	98.09	98.10	98.10	99.06	99.31
8	95.08	97.12	95.23	96.00	96.78	99.05	98.14	99.18
9	97.84	96.76	97.66	96.30	97.67	97.99	98.54	97.36
10	97.65	99.89	97.56	99.65	98.19	100.24	98.09	100.41
11	98.10	97.65	98.81	97.52	98.77	97.68	99.28	98.01
12	97.57	96.12	96.36	96.14	95.24	94.42	97.13	97.48
13	93.97	97.06	93.94	96.04	95.26	99.11	96.55	98.87
14	98.25	97.75	98.10	97.69	98.64	97.48	98.54	98.11
15	96.42	99.66	96.47	99.47	96.73	99.70	96.96	100.21
16	97.34	96.83	97.60	96.70	98.20	97.48	97.58	96.79
17	99.32	95.48	98.64	95.42	98.70	95.21	99.11	95.86
18	97.61	99.48	97.76	99.45	97.89	99.11	98.10	99.84
19	96.85	97.02	96.74	96.86	97.18	97.29	97.08	97.33
20	95.63	95.80	95.88	95.42	96.36	96.70	96.68	96.42
21	93.96	95.89	93.91	95.11	95.09	97.38	95.86	97.15
22	97.43	96.94	97.61	96.71	98.38	97.78	97.88	97.12
23	96.23	98.52	97.05	98.38	97.14	98.79	97.39	98.77
24	100.85	98.75	98.44	98.63	99.43	98.88	98.75	99.03
25	96.57	100.08	97.35	100.12	97.27	99.81	97.69	100.43
26	96.08	97.93	96.79	97.83	96.90	98.86	98.19	98.21
27	97.20	100.97	96.82	100.88	97.13	100.93	97.20	101.28
28	94.05	100.83	94.64	100.65	94.79	101.00	95.21	101.28

Table 6-1 (Continued)

29	97.62	100.20	97.60	100.12	97.72	100.02	98.00	100.53
30	96.31	99.09	96.65	99.00	96.42	98.81	97.11	99.53
31	96.16	100.82	97.72	100.64	96.71	100.83	97.29	101.29
32	95.43	101.20	96.11	100.96	96.39	100.97	96.83	101.72
33	97.08	101.49	97.57	101.43	97.31	101.00	98.05	102.00
34	97.52	96.43	97.54	96.35	97.41	96.32	97.91	96.76
35	97.78	98.73	98.73	98.58	99.08	98.99	99.12	98.94
36	97.30	95.69	97.65	95.62	97.77	95.66	97.98	95.95
37	97.88	96.45	98.51	96.34	98.68	96.47	98.92	96.80
38	96.36	99.77	97.40	99.56	97.79	100.05	97.80	100.02
Avg. % Error	3.03	2.19	2.84	2.41	2.56	2.04	2.15	1.86

6.4 CHEMICAL REACTION

The reactions involved in the dehydrogenation of sec-butanol on γ -alumina under the conditions of the present investigation were dehydrogenation (major), dehydration (minor) and decomposition (trace), as seen from the product distributions of all the experimental runs in Appendix V. The amount of methyl ethyl ketone was approximately equal to that of hydrogen. However the amount of total butene was consistently less than that of water. This was because dehydration was such a minor reaction that the quantity of water and butenes produced did not give a good analysis on the columns. The relation suggested that dehydrogenation and dehydration occurred in parallel as follows:



In addition to the above products, very trace amount of methane, diethyl ketone and n-propanol were also detected. Studying on the same reaction, it was reported (8) that at high temperatures ketone like intermediates were observed on the IR spectra which formed a stable carbohydrate surface structure accompanied by release of methane on heating to 300°C.

Diethyl ketone and n-propanol were detected as impurities in the sec-butanol feed.

6.5 THERMAL DECOMPOSITION

As mentioned in Section 5.2, sec-butanol remained unchanged when passed through Pyrex bed in the glass reactor at temperatures up to 447°C. This indicated that homogeneous thermal decomposition did not occur and the Pyrex surface was inert to sec-butanol decomposition under the experimental conditions of the present investigation.

6.6 EFFECT OF TIME ON CATALYTIC ACTIVITY

The choice of pure alumina as a catalyst was mentioned in Section 5.3. The activity of the alumina catalyst on both dehydrogenation and dehydration decreased with time of use due to the deposition of elemental carbon on the catalyst surface and probably the deactivation by water adsorption on the catalyst. The colour of the catalyst changed from an initial near white to light grey after 34 hours of use. To determine the effect of time on catalytic activity, samples were taken after 3 hours, 15 hours, 24 hours, 30 hours and 34 hours at constant conditions as mentioned in Section 5.5. The results are as shown in Figure 5-3. As can be observed the catalytic activity remained fairly constant all throughout this period. Samples were taken between 3 and 30 hours of operation on each batch of catalyst and therefore can be said to be well within the period of constant catalyst activity.

6.7 EFFECT OF SPACE VELOCITY AND FILM DIFFUSION

The effect of space velocity on product distribution is as shown in Appendix V and Figure 5-4.

When the gas film resistance is significant, the rate of reaction will be effected by the rate of flow of reactant to the surface of

the catalyst. In this case, the evaluation of the kinetic equation is complicated. Therefore it is important to first investigate if film resistance need be considered. In Figure 5-5 conversions are compared at given (space velocities)⁻¹ but different reactant flow rates. The conversion can be observed to be unaffected by the change in reactant flow rate at reaction temperature of 350°C and 1/S.V. of up to 60 gm.hr./mol. Since the experimental conditions for the kinetic evaluation for the present work is within these values, it can be assumed that film resistance is unimportant in all the experimental runs.

6.8 EFFECT OF PORE DIFFUSION

As mentioned in Section 5.8, if pore diffusion is significant, the size of the catalyst pellet should have an influence on the reaction rate or conversion. As shown in Table 5-1 under the same experimental conditions, run 37 was carried out using smaller particles of catalyst (14-20 mesh) and run 24 using larger catalyst particles (10-14 mesh). It can be observed that both particle sizes resulted in essentially the same sec-butanol conversion. It was concluded that pore diffusion did not play an important part in all the experimental runs.

6.9 KINETICS OF REACTION

As mentioned in Section 2.3, several types of models can be used for correlating reaction rate data. In this section, the advantages and disadvantages of the various methods will be discussed leading to a choice of method most suitable for the present work.

a) Choice of Correlation Method

A summary of the mechanistic approach for correlating reac-

tion rate data was outlined in Section 2.3.1. The equations derived by the Langmuir-Hinshelwood approach are adequate and are usually assumed to give an insight into the mechanism. However Bradshaw (43) recently re-emphasized that the basic assumption about single step rate controlling can be in substantial error. They revealed the presence of mutual rate controlling resistances for all catalytic steps of adsorption, surface reaction and desorption using Franckerts (44) data on dehydrogenation of ethanol. There is a lot of other evidence which indicates that the use of these equations is unjustified both theoretically and experimentally. One of the primary assumptions underlying the Langmuir-Hinshelwood theory is that no interaction occurs between adsorbed molecules, which implies that the heat of adsorption should be a constant, independent of the amount of gas adsorbed. Rhodin (45) showed that this condition is satisfied in practice only in extremely rare instances.

Another serious difficulty arises in the practical application of the Langmuir isotherm to the adsorption of a mixture of gases. The Langmuir equation predicts that the addition to one gas of a second gas will always decrease the amount of the first gas adsorbed. The opposite behavior was shown by Brunauer (46). This type of adsorption corresponds mathematically to having a negative adsorption coefficient in the denominator of the extended Langmuir equation. For example, when the adsorption of A is increased in the presence of B, the amount of A adsorbed is given by an expression of the form:

$$A_{\text{ads.}} = \frac{kp_A}{1 + K_A p_A - K_B p_B} \quad (6-3)$$

This is considered to be physically impossible in the Langmuir-Hinshelwood approach. Furthermore, their use has two unfortunate consequences: (1) because of the mathematical complexity of the differential rate expression, it is often very inconvenient to obtain the integral rate equation and to evaluate the numerous adjustable parameters, and (2) the investigator is often led to believe that he has uniquely deduced the mechanism of the reaction.

Besides, to find the mechanism, a very extensive experimental program would be required, using very precise and reproducible data because otherwise differences in fit may be so slight as to be explainable entirely in terms of experimental error. Also, if a number of alternative mechanisms fit the data equally well, it must be recognized that the equation selected is simply one of good fit, not one that represents reality. In the rate studies of the catalytic reaction of H_2S and SO_2 McGregor (47) illustrated the difficulty in finding the correct mechanism. Of the 27 rate expressions derived, at least ten were reported to correlate the data better than the rest. However no further model discrimination was attempted because none of the expressions could correlate the data better than the empirical rate expressions. It thus seems reasonable to employ the simplest possible rate equation which will adequately fit the experimental data.

The following expression for rate equations is suggested as being among the simplest forms having sufficient generality:

$$r = k (p_A)^m (p_B)^n (p_C)^0 \quad (6-4)$$

Weller (48) illustrated several examples where an equation of this form fits the data fully as well as a far more complicated one derived from the Langmuir theory. Data on synthesis of phosgene from carbon monoxide and chlorine over charcoal was correlated by Potter (49) by the equation:

$$r = \frac{k K_{CO} K_{Cl_2} p_{CO} p_{Cl_2}}{(1 + K_{Cl_2} p_{Cl_2} + K_{COCl_2} p_{COCl_2})^2} \quad (6-5)$$

where surface reaction between adsorbed CO and Cl₂ was the controlling step. The simplified equation:

$$r = k p_{CO} (p_{Cl_2})^{1/2} \quad (6-6)$$

correlated the data equally well over the experimental range.

Also, the reaction between methane and sulphur in the presence of silica gel catalyst undoubtedly has a true mechanism involving several physical and chemical steps. Yet over the experimental range of 550 to 700°C, Nabor and Smith (50) represent the data by the second-order rate equation:

$$r = k N_{CH_4} N_{S_2} \quad (6-7)$$

Clearly the constants of rate Equation (6-4) are more readily evaluated than those of equation derived by the mechanistic approach.

Commonly used methods for evaluating reaction rate constants from experimental data either presuppose a knowledge of the reaction

order or proceed by assuming an order in trial and error fashion (7, 10, 11, 12). This is the method of integrated equation as mentioned in Section 2.3.2. If, as frequently happens with complex and fractional order reaction, the correct assumption is not made on the first trial, the computations can become tedious. Very often, the method of fractional life times or the method of reference curves become impractical because of the requirement of large values of conversion such as 50 or 90%. At these high values of conversion, reactions are very often accompanied by side reactions. An alternative to all these methods is the differentiation method which was briefly described in Section 2.3.2. The main weak point to this method is the amount of error often present in kinetic data which makes it difficult to get sufficiently precise rate measurements. However with the advancement of digital computer models for data smoothing, the method of differentiation seems like a simple straight forward and reliable way for correlating kinetic data (33). Myint (33) presented a very good review on the various methods of data smoothing and differentiating techniques that can be used to obtain reaction rate data for use in the linear plot to determine reaction order and specific rate constant. The method of differentiation is therefore adopted for use in this work.

b) Method of Differentiation

The procedures involved in the method of differentiation as used in the present work shall be described below.

1. The rate of reaction for an integral plug-flow reactor is given by $\frac{dx}{d\tau}$ (10). This rate can be obtained by either graphically or numerically differentiating the conversion- $(SV)^{-1}$ data. Using the graphical method of fitting the data and

measurement of the slope is often unintentionally biased as well as tedious and is difficult to obtain precise rate data. The least squares method was used in smoothing the experimental data points.

A linear or non-linear function, which essentially has similar shape to that of the time-composition (conversion) data is fitted to the data. The parameters of the fitted function are determined by minimizing the residual of sum of squares. The resulting smooth function thus obtained is differentiated analytically. The numerical derivative $dx/d\tau$ at different time (1/S.V.) is now available.

2. A table of rates ($dx/d\tau$) versus concentrations is then prepared. Concentrations at various conversions can be prepared by the following expression considering volume expansion.

$$C_A = C_{A_0} \left(\frac{1 - X_A}{1 + \epsilon_A X_A} \right) \quad (6-8)$$

where C_{A_0} is the initial concentration of reactant and ϵ_A is the fractional change in volume of the system between no conversion and complete conversion (10). For example $A \rightarrow 4R$ with 50% inerts,

$$\epsilon_A = \frac{5 - 2}{2} = 1.5 \quad (6-9)$$

3. Now consider the rate equation

$$-\frac{dC_A}{d\tau} = -r_A = k C_A^n \quad (6-10)$$

Taking natural logarithm of both sides we have,

$$\ln(-r_A) = \ln(k) + n \ln(C_A) \quad (6-11)$$

A linear plot of some suitable simple functions of the reaction variables is made such that the two parameters of the line (slope and intercept) would uniquely determine the two constants (n and k) of the differential equation. The parameters of the fitted function were again determined by minimizing the residual of sum of squares.

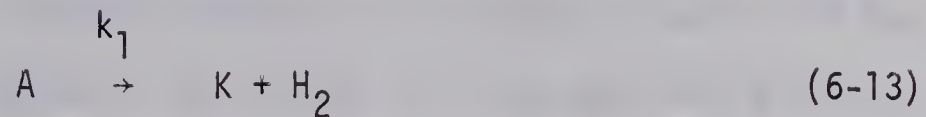
c) Application to Complex (Multi-Step) Reaction

The differential method has attractive features in analyzing complex reaction systems (33). Dalla Lana (6) suggested that the individual steps in multiple-step reaction system be modelled by considering the general form of rate equation as follows:

$$\frac{dC_i}{dt} = \sum_{j=1}^n r_{ij} (C_1, C_2, \dots, C_m) \quad (6-12)$$

in which the contributions to the overall rate of change of one component from each reaction step are summed. The individual terms in the right hand side of Equation (6-12), r_{ij} are each approximated by a power-law rate equation as determined by the method mentioned above.

Thus considering the parallel dehydrogenation and dehydration of sec-butanol we have:



where A = 2-butanol

K = methyl ethyl ketone

B = butenes

W = water

The rate equations are:

$$r_K = k_1 C_{A_K}^n = k_1 \left[C_{A_0} \left(\frac{1 - X_K}{1 + \epsilon_A X_K} \right) \right]^n \quad (6-15)$$

$$r_B = k_2 C_{A_B}^m = k_2 \left[C_{A_0} \left(\frac{1 - X_B}{1 + \epsilon_A X_B} \right) \right]^m \quad (6-16)$$

where X_K = conversion due to dehydrogenation

X_B = conversion due to dehydration

The overall rate of disappearance of 2-butanol is then given by:

$$(-r_A) = r_K + r_B \quad (6-17)$$

d) Kinetics of 2-butanol on NaOH doped Alumina

Using the Method of Differentiation, the data are fitted by the second degree polynomials as shown in Table 6-2 and 6-3 and Figure 6-1 for dehydrogenation and Table 6-6 and Figure 6-3 for

dehydration. These are done for the data obtained using the Coupled Reactor G.C. System. The natural logarithm of the rates and concentrations at various $1/S.V.$ are then calculated and shown in Tables 6-4 and 6-7. The least square method of the linear plot are done and shown in Table 6-5 and Figure 6-2 for dehydrogenation and Table 6-8 and Figure 6-4 for dehydration.

It can be observed that the correlation is good up to a total alcohol conversion of 12%. This was also reported by Chan (7) on 3-pentanol dehydrogenation, who attributed the bad correlation beyond 16% to the non-isothermal behavior in the catalyst bed. At high conversion, the endothermic effect of the reactions and the heat exchange nature of the reactor are believed to play a major role.

The constants thus evaluated from Figure 6-2 and Figure 6-4 are given below.

$$n \text{ (reaction order by dehydrogenation)} = 1.07$$

$$m \text{ (reaction order by dehydration)} = 1.60$$

$$k_1 \text{ (reaction rate constant by dehydrogenation)} = 2.891 \times 10^{-2} \frac{\text{liter fluid}}{(\text{hr})(\text{gm of cat})}$$

$$k_2 \text{ (reaction rate constant by dehydration)} = 0.913 \times 10^{-2} \frac{(\text{liter fluid})^{1.6}}{(\text{hr})(\text{gm of cat})(\text{mol})^{.6}}$$

Thus rate expressions can be written as below:

$$\text{Dehydrogenation: } r_K = 2.891 \times 10^{-2} \left[C_{A_0} \left(\frac{1 - X_K}{1 + \epsilon_A X_K} \right) \right]^{1.07} \quad (6-18)$$

$$\text{Dehydration: } r_B = 0.913 \times 10^{-2} \left[C_{A_0} \left(\frac{1 - X_B}{1 + \epsilon_A X_B} \right) \right]^{1.6} \quad (6-19)$$

The data obtained by the conventional method are treated in the same manner. The smoothed data are shown in Tables 6-10 and 6-13 and Figures 6-5 and 6-7. The calculated rates, concentrations and their natural logarithms are shown in Tables 6-11 and 6-14 and again the linear plots are done and shown in Tables 6-12 and 6-15 and Figures 6-6 and 6-8. The constants thus evaluated are shown as follows compared with those obtained by the coupled system.

Constant	Conventional System	Coupled Reactor GC System
n	1.3	1.07
m	2.1	1.60
k_1	3.667×10^{-2}	2.891×10^{-2}
k_2	2.560×10^{-2}	0.913×10^{-2}

As mentioned in Section 6.3, the material balance for the coupled system are generally better than those by the conventional system. Furthermore when Table 6-3 and Table 6-10 are compared the following can be observed.

	Coupled System	Conventional System
Maximum Percent Error	10.1	14.2
Variance	0.427	0.456

It is obvious that the coupled system is superior to the conventional system. Therefore it is more likely that the constant evaluated from the data obtained by the coupled system be more reliable. The order of reaction for dehydrogenation can be said to be of the

first order. It was reported that the dehydrogenation of 3-pentanol on 2N-NaOH doped Alundum, follows the first order as well (7).

The order of reaction for dehydration evaluated is 1.6. The extend of conversion due to dehydration reaction can be observed to be very minor (generally about 1% of dehydrogenation reaction). At this small conversion, accurate quantitative analysis of dehydration products are most difficult as was discussed in Section 6.4. Chan (7) reported that dehydration of 3-pentanol also follows the first order. However the catalyst used was Alundum which consists of 21% SiO_2 . SiO_2 is more dehydrating because of the increase covalent character (17). This was observed in Chan's results where dehydration reaction was generally about 4% that of dehydrogenation as compared to 1% for the present work. Hence it can be concluded that 2-butanol, on 2N-NaOH doped γ -alumina was converted almost solely by dehydrogenation reaction.

There was not enough data available to attempt correlation by the mechanistic approach. However, it would be interesting to compare results obtained by this work with those using the mechanistic approach. Chan (7) and Chuang (14) worked on the same reaction but with different alcohols.

Chan reported that dehydrogenation of 3-pentanol at 370°C involves a single site mechanism with chemisorption of ketone and adsorption of alcohol rate controlling. The proposed rate expression was:

$$r_K = \frac{k_1 p_A}{(1 + K_K p_K)} \quad (6-20)$$

in which at low conversion, $K_K p_K$ would become negligible so that the expression would become,

$$r_K = k_1 p_A \quad (6-21)$$

which is in agreement with the present work.

The reaction rate expression that was proposed by Chuang for the dehydrogenation of 2-propanol on 8% NaOH doped alumina is given below.

$$(-r_A) = \frac{b_1 p_A}{\sqrt{p_{H_2}} (1 + b_2 p_A / \sqrt{p_{H_2}} + b_3 \sqrt{p_{H_2}})} \quad (6-22)$$

In the above expression, within the present experimental conditions, the term $(1 + b_2 p_A / \sqrt{p_{H_2}} + b_3 \sqrt{p_{H_2}})$ is nearly constant. Therefore Equation (6-22) can be reduced to give the following expression.

$$(-r_A) = \frac{b p_A}{\sqrt{p_{H_2}}} \quad (6-23)$$

Tables 6-16 and 6-17 and Figure 6-9 show that the present data correlate the reduced expression well.

The rate expression derived by the correlation is

$$(-r_A) = \frac{k_1 C_A^{1.04}}{\sqrt{C_{H_2}}} \quad (6-24)$$

Thus it can be observed that the empirical approach taken in this work fits the data fully as well as the far more complicated one derived from the Langmuir theory, under the experimental conditions.

TABLE 6-2
DATA CORRELATION FOR COUPLED SYSTEM

1/S.V.	Run No.	ϵ_A	C_{A_O}	X_K	X_B	Material Balance
9.81	27	.90489	.03393	6.8573	0.0593	96.63
13.31	28	.86981	.03227	7.4768	0.0909	100.83
13.31	29	.86875	.03214	7.2291	0.0927	100.20
14.75	34	.89280	.03369	8.4370	0.0807	96.43
14.75	36	.89191	.03322	7.5791	0.0750	95.69
19.97	35	.86402	.03230	9.0150	0.1042	98.73
20.00	24	.82029	.02961	11.3858	0.1674	98.75
26.61	25	.79350	.02817	13.3479	0.1735	100.08
26.61	30	.79017	.02780	11.2928	0.1772	99.09
30.00	33	.82150	.02993	14.0681	0.2315	101.49
39.92	31	.79017	.02770	15.4971	0.3046	100.82
39.97	26	.74103	.02466	15.6216	0.2490	97.93
59.96	32	.73701	.02461	18.4153	0.2941	101.21

TABLE 6-3

POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR
DEHYDROGENATION IN A COUPLED SYSTEM

X = 1/SV GM HR/MOL
Y = CONVERSION PERCENT

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 1.64582

A1 = 0.50527

A2 = -0.00378

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
0.00000	0.00000	1.64582	
9.81000	6.85730	6.23865	9.02164
13.31000	7.47680	7.70111	3.00007
13.31000	7.22910	7.70111	6.52931
14.75000	8.43700	8.27590	1.90938
14.75000	7.57910	8.27590	9.19375
19.97000	9.61500	10.22805	6.37600
20.00000	11.38580	10.23867	10.07503
26.61000	13.34790	12.41343	7.00084
26.61000	11.29280	12.41343	9.92344
30.00000	14.06810	13.40057	4.74493
39.97000	15.62160	15.80004	1.14226
39.92000	15.49710	15.78988	1.88928
59.96000	18.41530	18.34611	0.37572

VARIANCE = 0.427385

STANDARD DEVIATION = 0.653747

MAXIMUM PCT ERROR = 10.075037

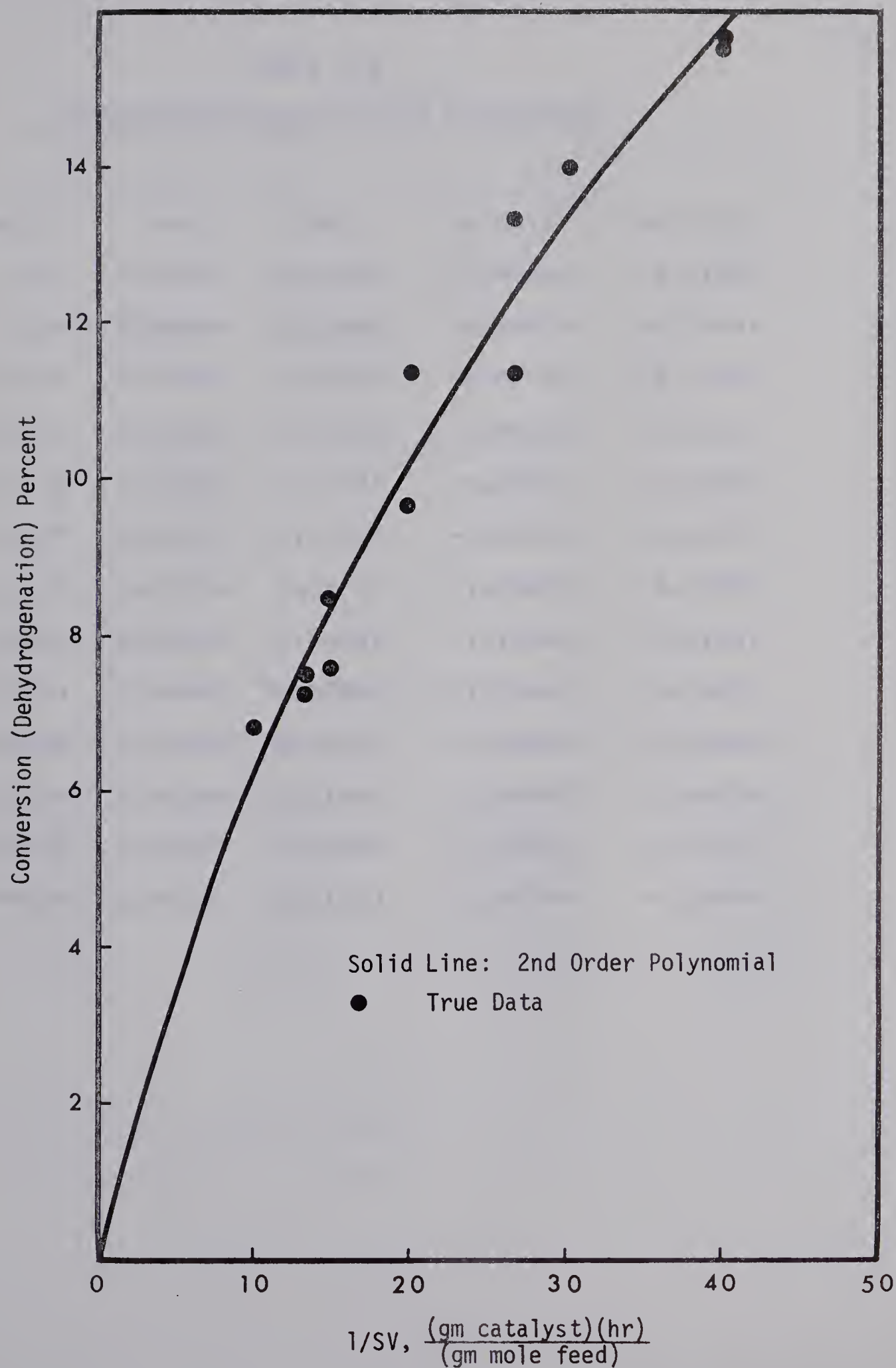


FIGURE 6-1 POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR COUPLED SYSTEM

TABLE 6-4

DEHYDROGENATION REACTION PARAMETERS

1/S.V.	RATE	CONC.	LN RATE	LN CONC.
9.81	0.43110	0.02975	-0.84140	-3.51469
13.31	0.40464	0.02803	-0.90474	-3.57433
13.31	0.40464	0.02805	-0.90474	-3.57360
14.75	0.39375	0.02868	-0.93201	-3.55132
14.75	0.39375	0.02875	-0.93201	-3.54883
19.97	0.35429	0.02695	-1.03762	-3.61358
20.00	0.35406	0.02399	-1.03826	-3.72980
26.61	0.30409	0.02207	-1.19040	-3.81343
26.61	0.30409	0.02264	-1.19040	-3.78802
30.00	0.27846	0.02305	-1.27844	-3.76987
39.97	0.20309	0.01864	-1.59407	-3.98196
39.92	0.20347	0.02085	-1.59221	-3.87022
59.96	0.05197	0.01767	-2.95704	-4.03539

TABLE 6-5

STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES)
FOR DEHYDROGENATION IN A COUPLED SYSTEM

X = LN CONC
Y = LN RATE

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 2.89073

A1 = 1.06972

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
-3.51469	-0.84140	-0.86902	3.28325
-3.57433	-0.90474	-0.93282	3.10407
-3.57360	-0.90474	-0.93204	3.01775
-3.55132	-0.93201	-0.90820	2.55372
-3.54883	-0.93201	-0.90554	2.83951
-3.61358	-1.03762	-0.97481	6.05321
-3.72980	-1.03826	-1.09913	5.86310
-3.81343	-1.19040	-1.18859	0.15157
-3.78802	-1.19040	-1.16141	2.43499

VARIANCE = 0.001507

STANDARD DEVIATION = 0.038823

MAXIMUM PCT ERROR = 6.053214

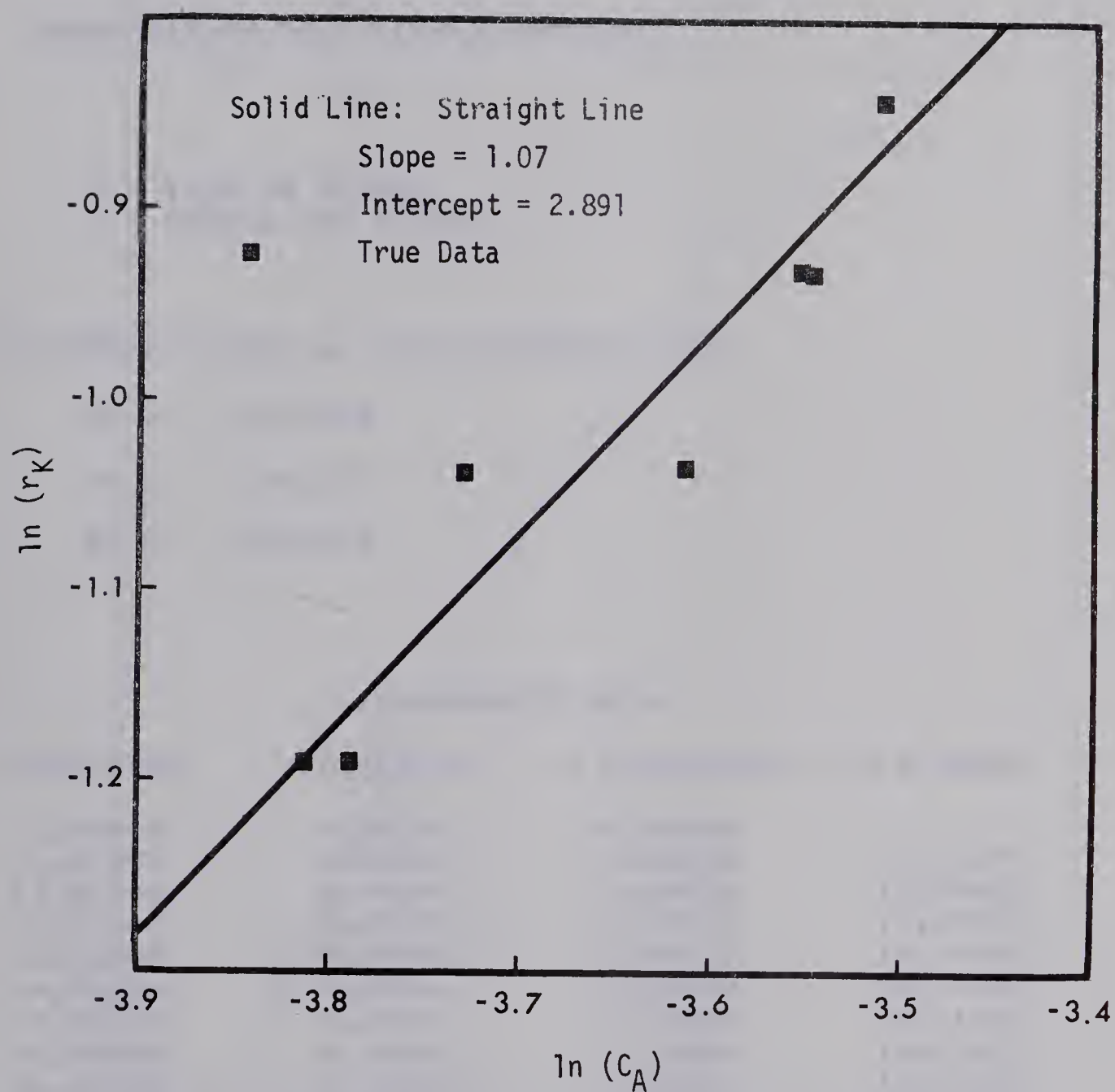


FIGURE 6-2. STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES) FOR COUPLED SYSTEM

TABLE 6-6

POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR
DEHYDRATION IN A COUPLED SYSTEM

X = 1/SV GM HR/MOL
Y = CONVERSION PERCENT

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = -0.07090

A1 = 0.01277

A2 = -0.00010

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
0.00000	0.00000	-0.07090	
9.81000	0.05930	0.04390	25.96375
13.31000	0.09090	0.07976	12.25437
13.31000	0.09270	0.07976	13.95817
14.75000	0.08070	0.09373	16.15155
14.75000	0.07500	0.09373	24.97908
19.97000	0.10420	0.14058	34.91392
20.00000	0.16740	0.14083	15.87077
26.61000	0.17350	0.19154	10.40006
26.61000	0.17720	0.19154	8.09486
30.00000	0.23150	0.21383	7.62898
39.97000	0.24900	0.26481	6.35264
39.92000	0.30460	0.26461	13.12644
59.96000	0.29410	0.30143	2.49312

VARIANCE = 0.000448

STANDARD DEVIATION = 0.021167

MAXIMUM PCT ERROR = 34.913925

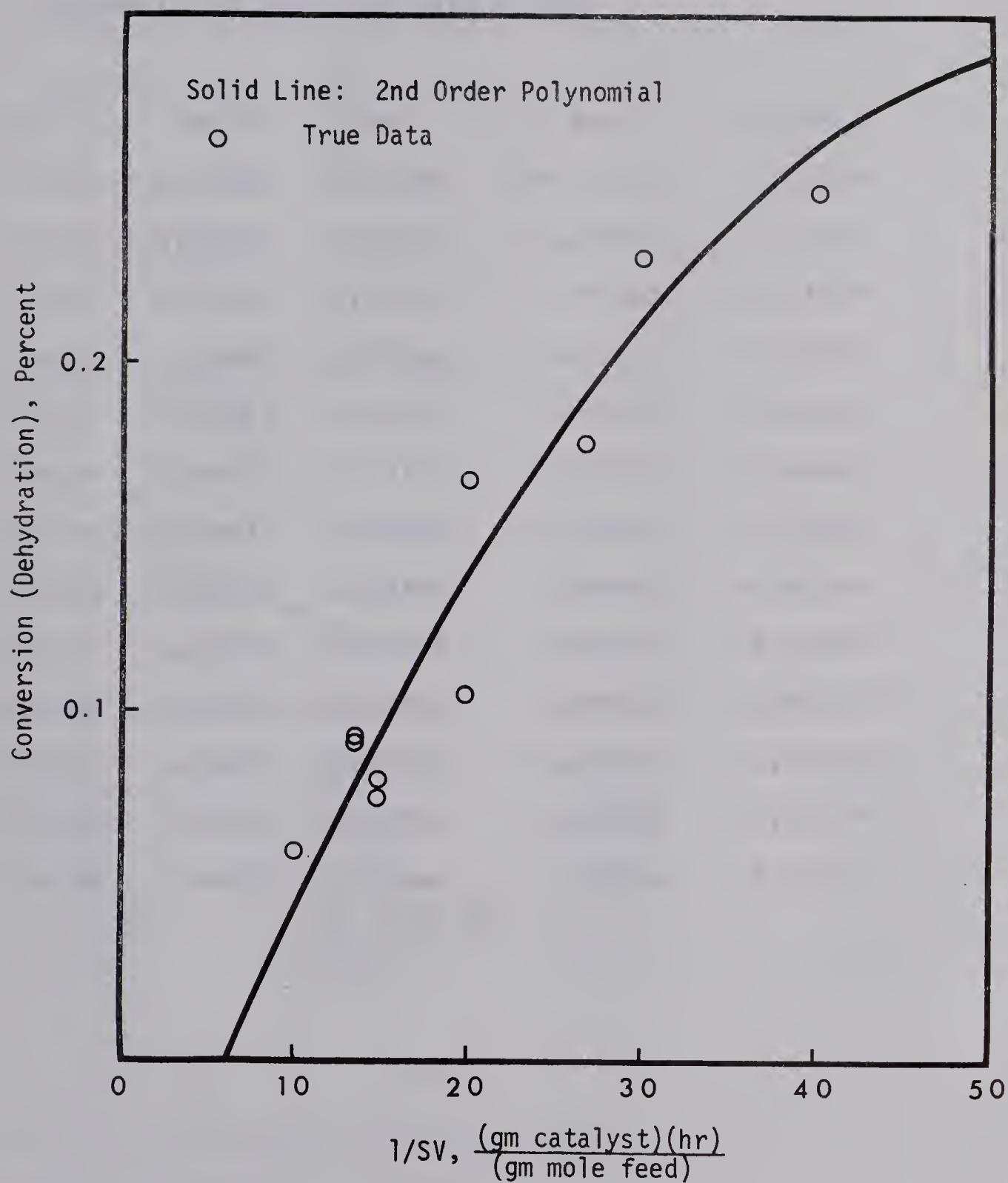


FIGURE 6-3. POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR COUPLED SYSTEM

TABLE 6-7

DEHYDRATION REACTION PARAMETERS

1/S.V.	RATE	CONC.	LN RATE	LN CONC.
9.81	0.01080	0.03389	-4.52746	-3.38458
13.31	0.01010	0.03221	-4.59442	-3.43531
13.31	0.01010	0.03208	-4.59442	-3.43938
14.75	0.00981	0.03363	-4.62333	-3.39208
14.75	0.00981	0.03317	-4.62333	-3.40602
19.97	0.00877	0.03223	-4.73573	-3.43463
20.00	0.00877	0.02951	-4.73641	-3.52269
26.61	0.00744	0.02808	-4.89980	-3.57260
26.61	0.00744	0.02771	-4.89980	-3.58589
30.00	0.00676	0.02980	-4.99525	-3.51311
39.97	0.00477	0.02455	-5.34415	-3.70690
39.92	0.00478	0.02754	-5.34206	-3.59177
59.96	0.00077	0.02448	-7.15878	-3.70971

TABLE 6-8

STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES)
FOR DEHYDRATION IN A COUPLED SYSTEM

X = LN CONC
Y = LN RATE

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 0.91335

A1 = 1.61853

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
-3.38458	-4.52746	-4.56470	0.82270
-3.43531	-4.59442	-4.64681	1.14042
-3.43938	-4.59442	-4.65340	1.28381
-3.39208	-4.62333	-4.57684	1.00540
-3.40602	-4.62333	-4.59940	0.51739
-3.43463	-4.73573	-4.64571	1.90075
-3.52269	-4.73641	-4.78824	1.09437
-3.57260	-4.89980	-4.86902	0.62808
-3.58589	-4.89980	-4.89053	0.18908

VARIANCE = 0.002770

STANDARD DEVIATION = 0.052639

MAXIMUM PCT ERROR = 1.900751

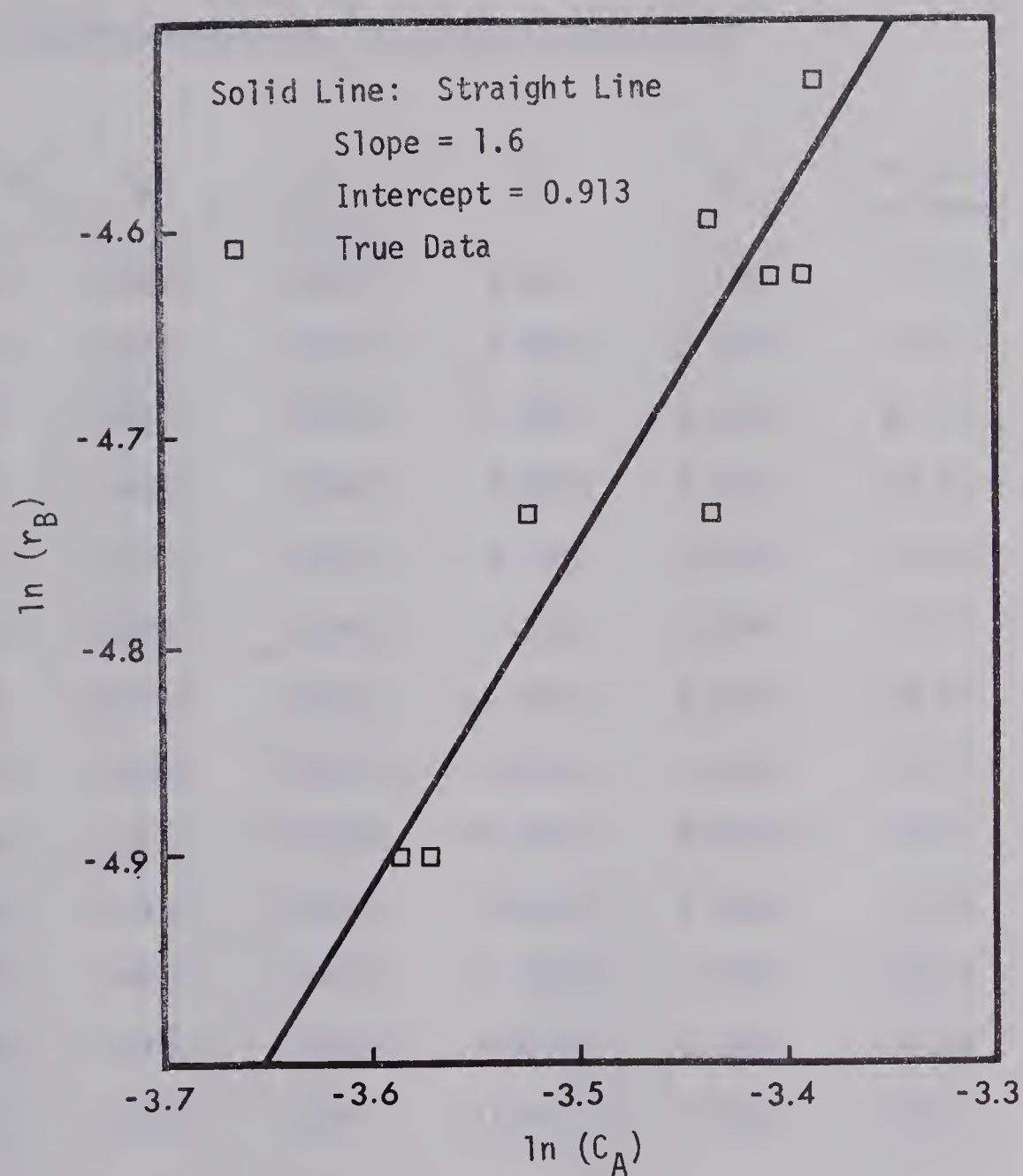


FIGURE 6-4. STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES) FOR COUPLED SYSTEM

TABLE 6-9

DATA CORRELATION FOR CONVENTIONAL SYSTEM

1/S.V.	Run No.	ϵ_A	C_{A_0}	X_K	X_B	Material Balance
9.81	27	.90489	.03393	6.3007	0.1328	97.20
13.31	28	.86981	.03227	7.5444	0.1682	94.05
13.31	29	.86875	.03214	6.3242	0.1502	97.62
14.75	34	.89280	.03369	6.9742	0.1374	97.52
14.75	36	.89191	.03322	6.5164	0.1560	97.30
19.97	35	.86402	.03230	8.1247	0.1595	97.78
20.00	24	.82029	.02961	10.3355	0.2872	100.85
26.61	25	.79350	.02817	11.4923	0.2329	96.57
26.61	30	.79017	.02780	10.7090	0.2404	96.31
30.00	33	.82150	.02993	12.0994	0.3087	97.08
39.92	31	.79017	.02770	14.9568	0.3593	96.16
39.97	26	.74103	.02466	14.1761	0.3024	96.08
59.96	32	.73701	.02461	15.4574	0.3589	95.43

TABLE 6-10

POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR
DEHYDROGENATION IN A CONVENTIONAL SYSTEM

X = 1/SV GM HR/MOL
Y = CONVERSION PERCENT

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 0.85917

A1 = 0.50563

A2 = -0.00431

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
0.00000	0.00000	0.85917	
9.81000	6.30070	5.40459	14.22224
13.31000	7.54440	6.82551	9.52870
13.31000	6.32420	6.82551	7.92694
14.75000	6.97420	7.37946	5.81086
14.75000	6.51640	7.37946	13.24444
19.97000	8.12470	9.23766	13.69851
20.00000	10.33550	9.24766	10.52525
26.61000	11.49230	11.26191	2.00468
26.61000	10.70900	11.26191	5.16307
30.00000	12.09940	12.14882	0.40846
39.97000	14.17610	14.18310	0.04937
39.92000	14.95680	14.17504	5.22678
59.96000	15.45740	15.68043	1.44290

VARIANCE = 0.455728

STANDARD DEVIATION = 0.675076

MAXIMUM PCT ERROR = 14.222248

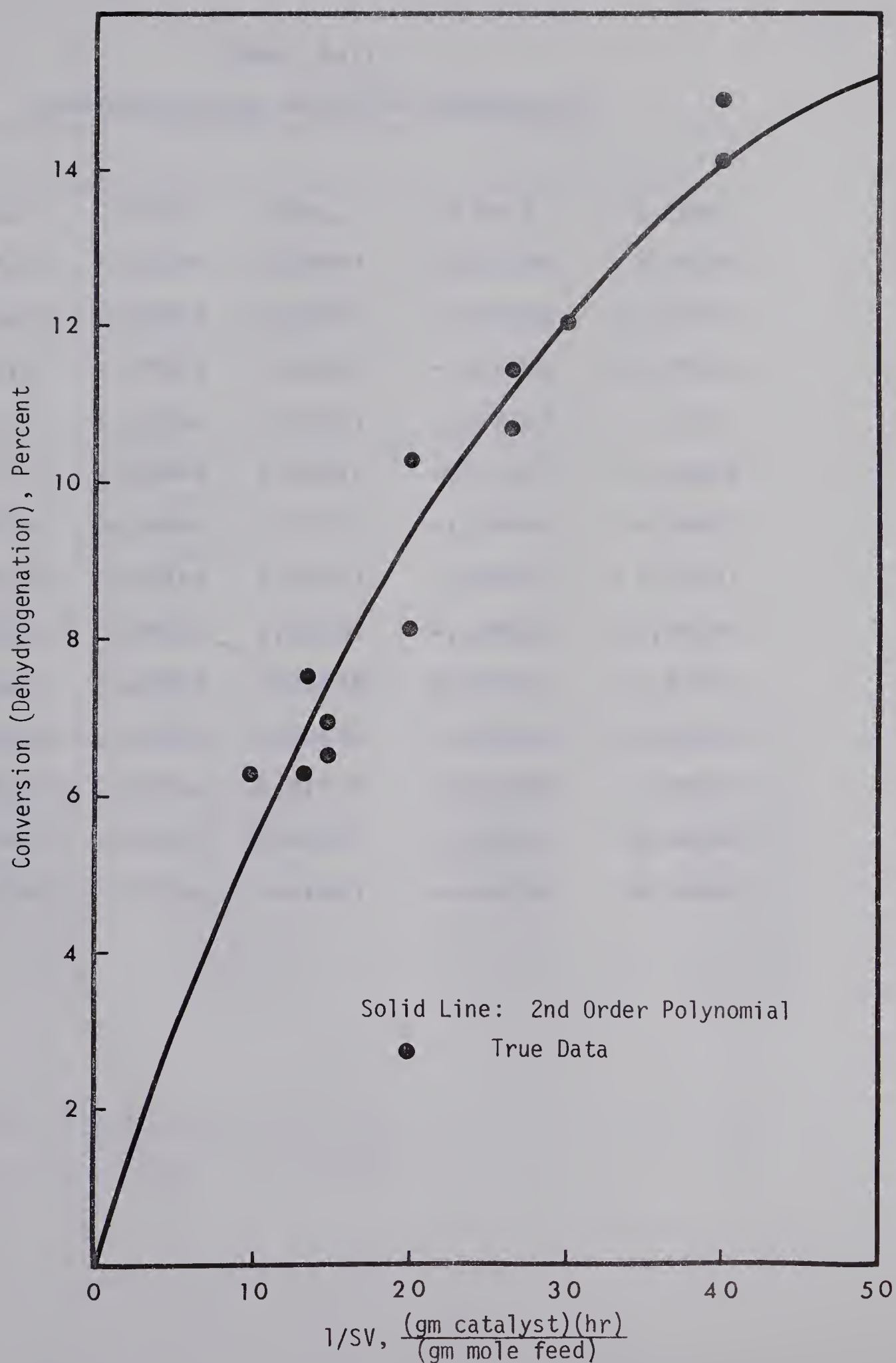


FIGURE 6-5. POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR CONVENTIONAL SYSTEM

TABLE 6-11

DEHYDROGENATION REACTION PARAMETERS

1/S.V.	RATE	CONC.	LN RATE	LN CONC.
9.81	0.42106	0.03007	-0.86496	-3.50398
13.31	0.39089	0.02799	-0.93930	-3.57561
13.31	0.39089	0.02853	-0.93930	-3.55646
14.75	0.37848	0.02950	-0.97157	-3.52325
14.75	0.37848	0.02934	-0.97157	-3.52848
19.97	0.33348	0.02772	-1.09814	-3.58527
20.00	0.33322	0.02447	-1.09892	-3.71011
26.61	0.27625	0.02284	-1.28644	-3.77884
26.61	0.27625	0.02288	-1.28644	-3.77721
30.00	0.24702	0.02393	-1.39824	-3.73261
39.97	0.16108	0.01915	-1.82580	-3.95533
39.92	0.16151	0.02106	-1.82312	-3.86003
59.96	-0.01122	0.01867	-4.48958	-3.98035

TABLE 6-12

STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES)
FOR DEHYDROGENATION IN A CONVENTIONAL SYSTEM

X = LN CONC
Y = LN RATE

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 3.66739

A1 = 1.30498

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
-3.50398	-0.86496	-0.90524	4.65788
-3.57561	-0.93930	-0.99872	6.32650
-3.55646	-0.93930	-0.97373	3.66600
-3.52325	-0.97157	-0.93039	4.23790
-3.52848	-0.97157	-0.93722	3.53542
-3.58527	-1.09814	-1.01133	7.90504
-3.71011	-1.09892	-1.17424	6.85450
-3.77884	-1.28644	-1.26393	1.74925
-3.77721	-1.28644	-1.26181	1.91459

VARIANCE = 0.002942

STANDARD DEVIATION = 0.054242

MAXIMUM PCT ERROR = 7.905045

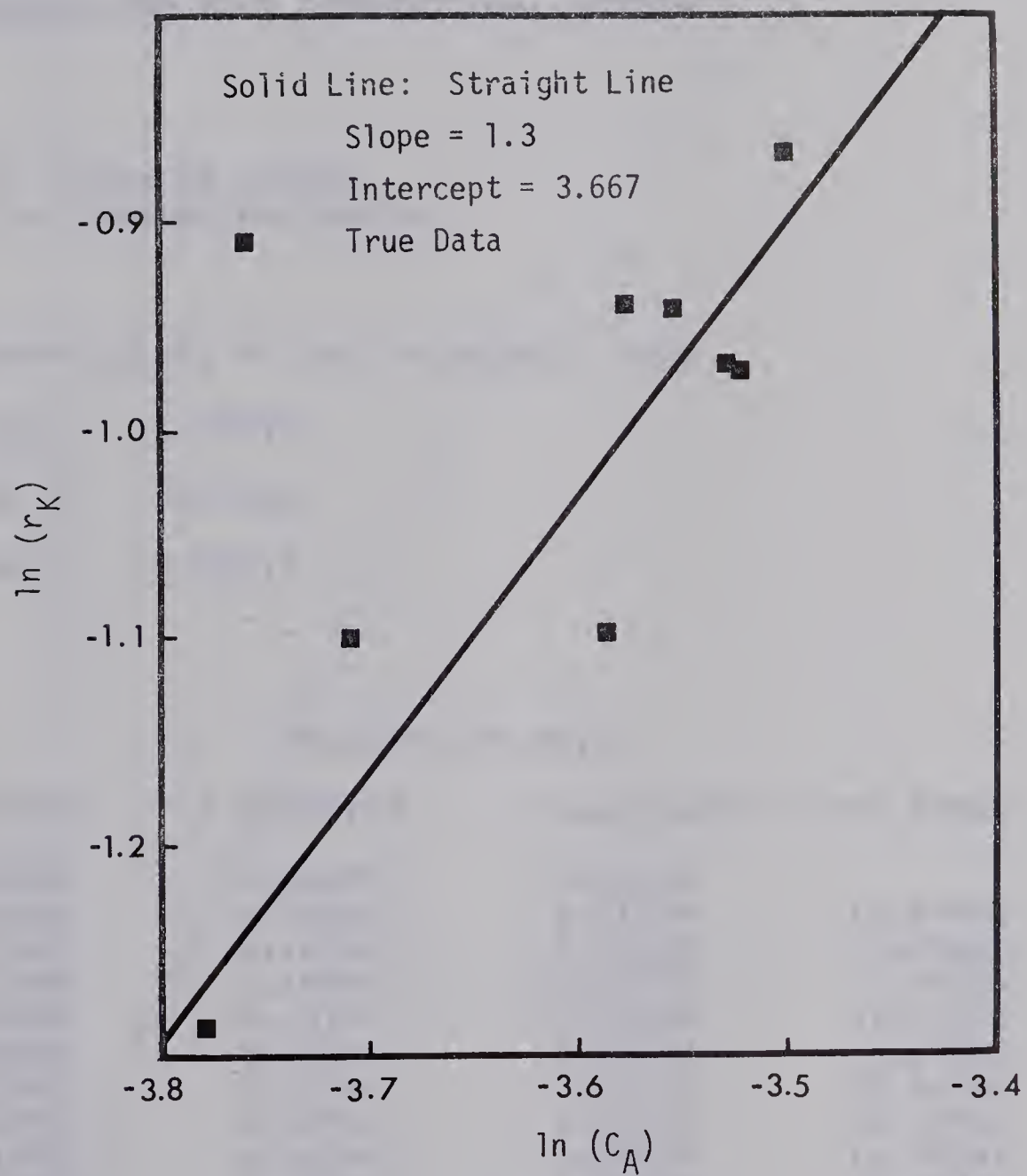


FIGURE 6-6. STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES) FOR CONVENTIONAL SYSTEM

TABLE 6-13

POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR
DEHYDRATION IN A CONVENTIONAL SYSTEM

X = 1/SV GM HR/MOL
Y = CONVERSION PERCENT

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 0.00270

A1 = 0.01286

A2 = -0.00012

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
0.00000	0.00000	0.00270	
9.81000	0.13280	0.11739	11.59861
13.31000	0.16820	0.15272	9.20018
13.31000	0.15020	0.15272	1.68129
14.75000	0.13740	0.16640	21.11106
14.75000	0.15600	0.16640	6.67088
19.97000	0.15950	0.21182	32.80788
20.00000	0.28720	0.21207	26.15922
26.61000	0.23290	0.26015	11.70238
26.61000	0.24040	0.26015	8.21749
30.00000	0.30870	0.28074	9.05521
39.97000	0.30240	0.32531	7.57927
39.92000	0.35930	0.32515	9.50300
59.96000	0.33890	0.34280	1.15320

VARIANCE = 0.001033

STANDARD DEVIATION = 0.032149

MAXIMUM PCT ERROR = 32.807884

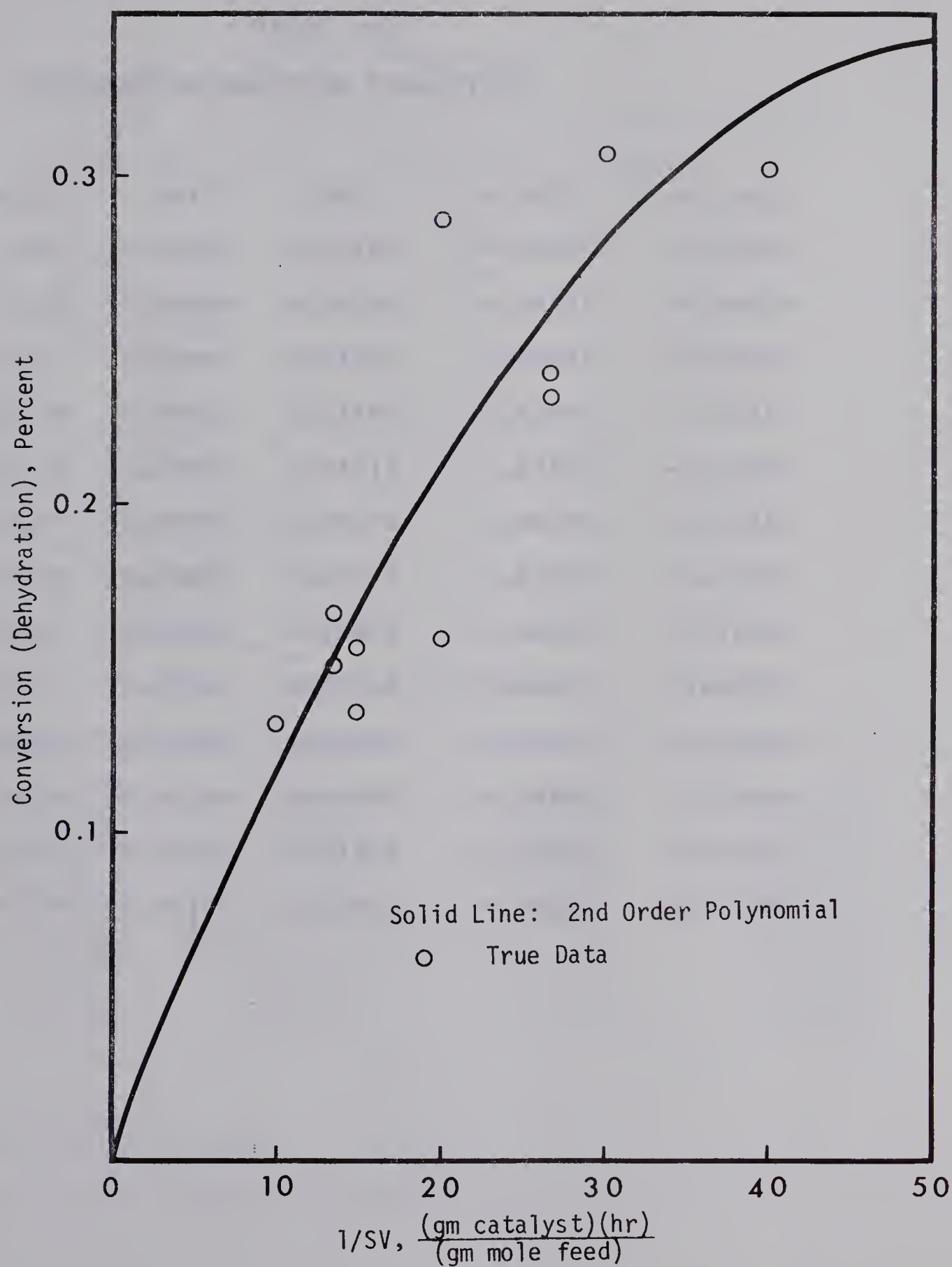


FIGURE 6-7. POLYNOMIAL APPROXIMATION (LINEAR LEAST SQUARES) FOR CONVENTIONAL SYSTEM

TABLE 6-14

DEHYDRATION REACTION PARAMETERS

1/S.V.	RATE	CONC.	LN RATE	LN CONC.
9.81	0.01050	0.03384	-4.55584	-3.38598
13.31	0.00966	0.03216	-4.63918	-3.43676
13.31	0.00966	0.03204	-4.63918	-3.44046
14.75	0.00932	0.03360	-4.67559	-3.39315
14.75	0.00932	0.03312	-4.67559	-3.40755
19.97	0.00806	0.03220	-4.81994	-3.43566
20.00	0.00805	0.02945	-4.82084	-3.52487
26.61	0.00647	0.02805	-5.04002	-3.57367
26.61	0.00647	0.02768	-5.04002	-3.58702
30.00	0.00565	0.02976	-5.17433	-3.51451
39.97	0.00326	0.02453	-5.72382	-3.70783
39.92	0.00327	0.02752	-5.72015	-3.59275
59.96	-0.00153	0.02446	-6.48222	-3.71049

TABLE 6-15

STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES)
FOR DEHYDRATION IN A CONVENTIONAL SYSTEM

X = LN CONC
Y = LN RATE

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 2.56021

A1 = 2.11473

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
-3.38598	-4.55584	-4.60022	0.97420
-3.43676	-4.63918	-4.70761	1.47504
-3.44046	-4.63918	-4.71543	1.64369
-3.39315	-4.67559	-4.61538	1.28763
-3.40755	-4.67559	-4.64583	0.63632
-3.43566	-4.81994	-4.70528	2.37879
-3.52487	-4.82084	-4.89393	1.51629
-3.57367	-5.04002	-4.99713	0.85084
-3.58702	-5.04002	-5.02536	0.29069

VARIANCE = 0.004689

STANDARD DEVIATION = 0.068483

MAXIMUM PCT ERROR = 2.378794

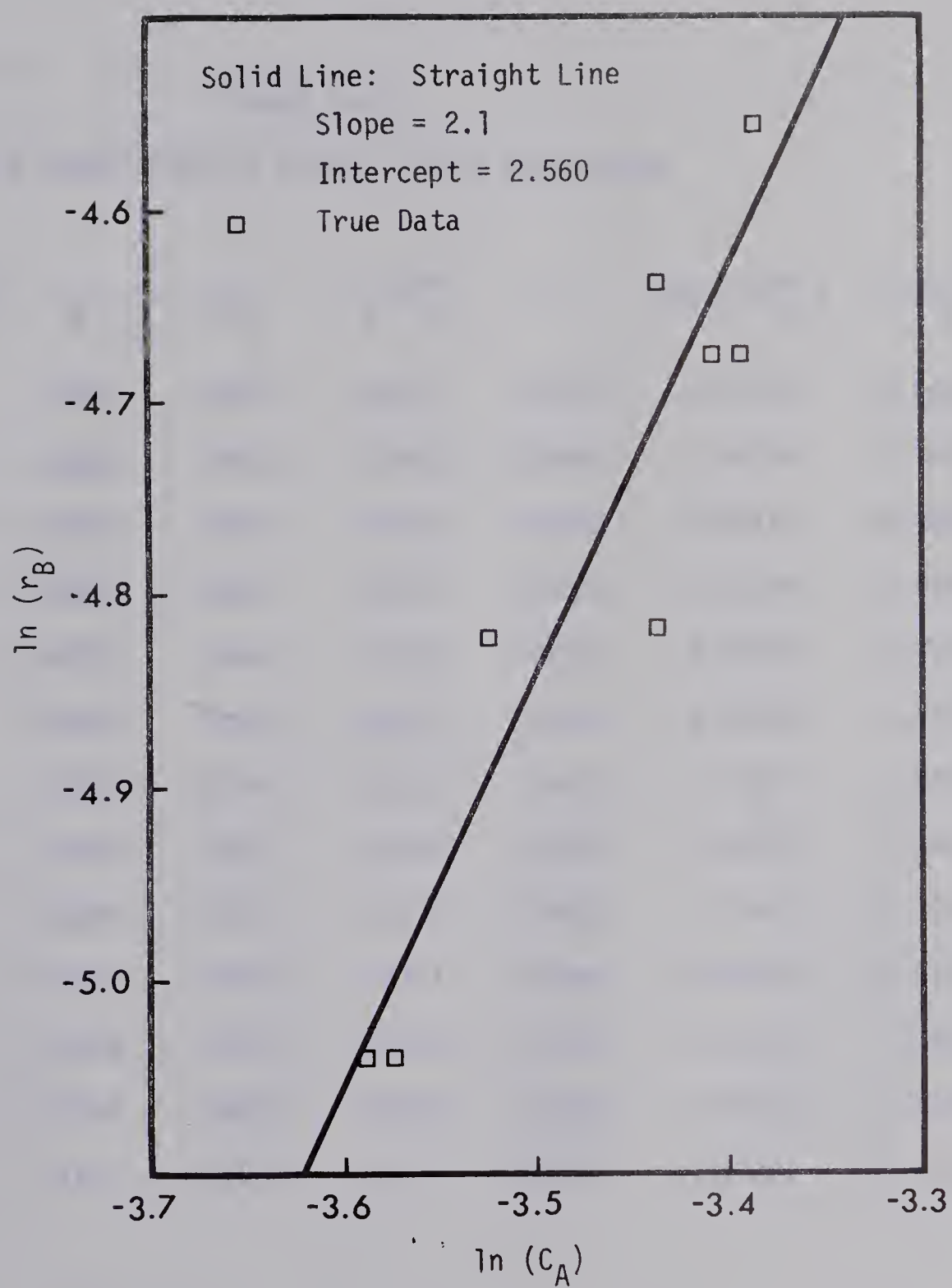


FIGURE 6-8. STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES) FOR CONVENTIONAL SYSTEM

TABLE 6-16

DATA CORRELATION TO CHUANG'S RATE EXPRESSION

1/S.V.	Run No.	C_A	C_{H_2}	$C_A/\sqrt{C_{H_2}}$	r_K	$\ln(C_A/\sqrt{C_{H_2}})$	$\ln(r_K)$
9.81	27	.02975	.00418	.46017	.43110	-0.77615	-0.84141
13.31	28	.02803	.00424	.43050	.40464	-0.84280	-0.90475
13.31	29	.02805	.00409	.43862	.40464	-0.82412	-0.90475
14.75	34	.02868	.00501	.40519	.39375	-0.90339	-0.93203
14.75	36	.02875	.00447	.43006	.39375	-0.84383	-0.93203
19.97	35	.02695	.00535	.36847	.35429	-0.99839	-1.03763
20.00	24	.02399	.00562	.32003	.35406	-1.13934	-1.03828
26.61	25	.02207	.00610	.28258	.30409	-1.26379	-1.19043
26.61	30	.02264	.00516	.31518	.30409	-1.15461	-1.19043
30.00	33	.02305	.00688	.27791	.27846	-1.28045	-1.27848
39.92	31	.02085	.00685	.25193	.20347	-1.37860	-1.59223
39.97	26	.01864	.00602	.24026	.20309	-1.42603	-1.59410
59.96	32	.01767	.00694	.21212	.05197	-1.55060	-2.95708

TABLE 6-17

STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES)
FOR DEHYDROGENATION REACTION

$$X = \ln(CA/RTCH_2)$$

$$Y = \ln \text{ RATE}$$

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

$$A_0 = -0.01933$$

$$A_1 = 1.04329$$

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
-0.77615	-0.84141	-0.82908	1.46428
-0.84280	-0.90475	-0.89862	0.67697
-0.82412	-0.90475	-0.87913	2.83103
-0.90339	-0.93203	-0.96183	3.19823
-0.84383	-0.93203	-0.89969	3.46880
-0.99839	-1.03763	-1.06095	2.24763
-1.15461	-1.19043	-1.22393	2.81460
-1.28045	-1.27848	-1.35522	6.00281
-1.42603	-1.59410	-1.50710	5.45712

$$\text{VARIANCE} = 0.002237$$

$$\text{STANDARD DEVIATION} = 0.047306$$

$$\text{MAXIMUM PCT ERROR} = 6.002817$$

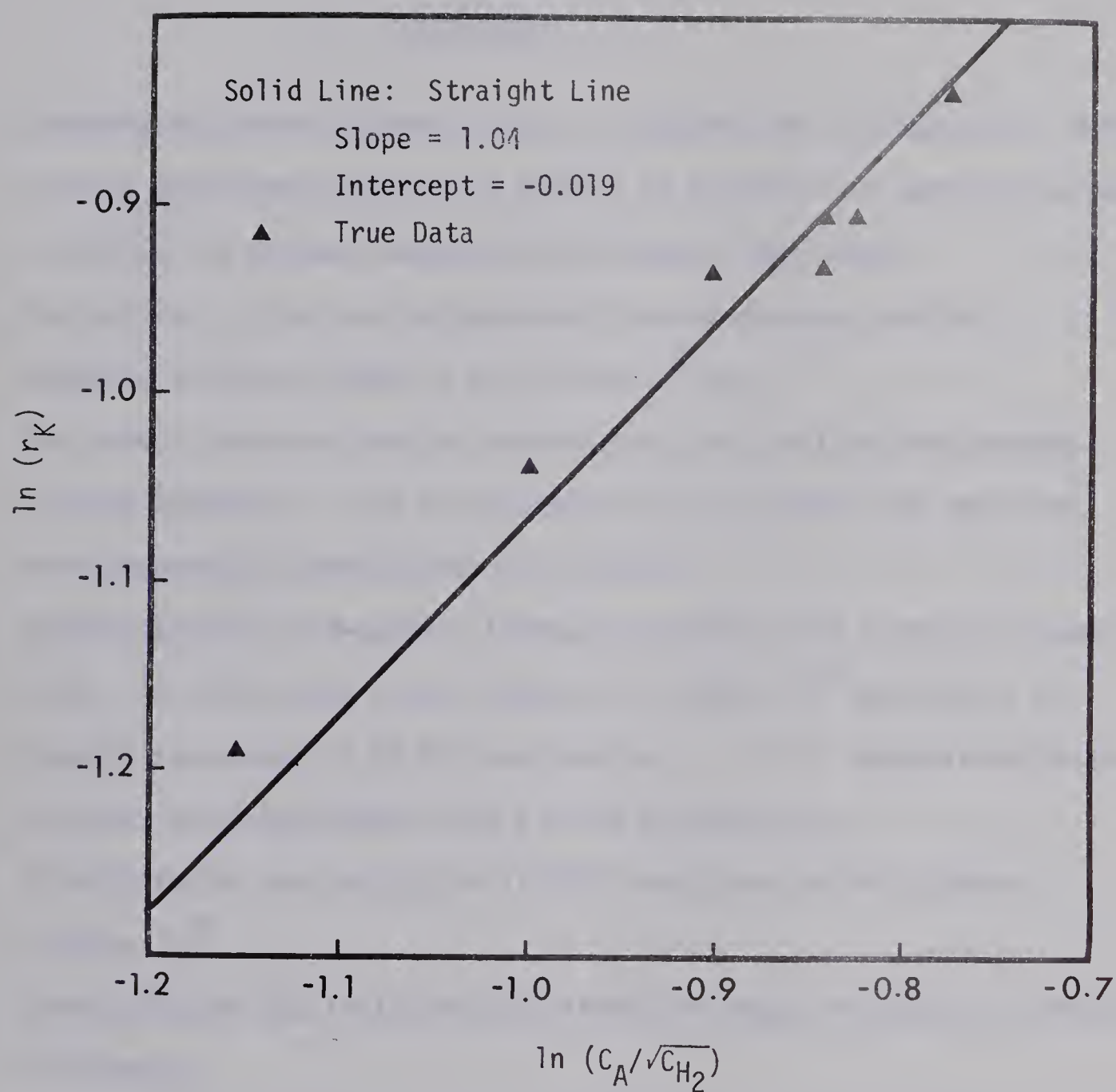


FIGURE 6-9. STRAIGHT LINE APPROXIMATION (LINEAR LEAST SQUARES) FOR CHUANG'S RATE EXPRESSION

CHAPTER 7

CONCLUSIONS

1. Homogeneous thermal decomposition of 2-butanol was not detected. Pyrex surface exhibited no catalytic effects on 2-butanol at temperatures up to 447°C, the maximum temperature employed in this study.
2. The activity of the sodium hydroxide treated alumina catalyst remained constant between 3 to 34 hours of use.
3. The sodium hydroxide treated alumina catalyst catalyzed dehydrogenation of 2-butanol. Very minor dehydration and other side reactions were observed at temperatures up to 350°C.
4. Dehydrogenation of 2-butanol increased markedly with increasing temperature. At 414°C and a space velocity of 2.468×10^{-2} mol/g.hr., 2-butanol conversion of 69.29% was obtained. At this temperature dehydration was quite noticeable with a 2.01% butene yield.
5. Film diffusion was negligible at 350°C and space velocity above 1.667×10^{-2} .
6. Pore diffusion was insignificant within the range of catalytic particles 10-20 mesh.
7. The material balances for the coupled reactor-G.C. system were generally better than that for the conventional system by about an average of 1%.
8. A first order rate expression was found to fit the data well for the dehydrogenation of 2-butanol on 2N-NaOH treated alumina under the experimental conditions.

CHAPTER 8

NOTES AND RECOMMENDATIONS

1. The microfeeder used provided very accurate feed rate with maximum error of less than 0.5%.
2. The mass flow meter was accurate with maximum error of 0.4%. However, to improve the material balance further, a flow meter with larger range of flow rate (about 90% of total feed) would be desirable.
3. The temperature control for the vaporizer, reactor and other heating systems was good and adequate for future kinetics studies.
4. The chromatographic analytical methods used in the present investigation were sufficient. The relative response factors given by Kaiser are quite accurate for most components. The factor for water at very low concentration should be verified.
5. A tie-in line from the line between the vaporizer outlet and the reaction inlet to the direct sampling valve could be constructed to provide an analysis of the feed composition. This will provide another way to check the accuracy of the final analysis.

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NOMENCLATURE

A	Alcohol
A_{ads}	Amount of A adsorbed
B	Butenes
b_i	Arbitrary constant of i^{th}
C_A	Concentration of component A; mol per liter
C_{A_0}	Initial concentration of component A; mol per liter
C_i	Concentration of i^{th} component; mol per liter
ϵ_A	Fractional change in volume on reaction
f_i	Relative response factor of i^{th} component
K	Ketone
K_A	Adsorption constant of component A
K_B	Adsorption constant of component B
K_C	Adsorption constant of component C
k	Reaction rate constant
k_1	Reaction rate constant for dehydrogenation
k_2	Reaction rate constant for dehydration
m	Order of reaction
N_i	Moles of component i
n	Order of reaction
o	Order of reaction
p_A	Partial pressure of component A
p_B	Partial pressure of component B
p_C	Partial pressure of component C
r, r_A	Rate of reaction; g mol of reactant converted per hour per gm of catalyst
r_K	Rate of dehydrogenation reaction

r_B	Rate of dehydration reaction
t	Reaction time
W	Water
$x_{A,x}$	Conversion; mol of alcohol converted per mol of alcohol fed
x_K	Conversion due to dehydrogenation
x_B	Conversion due to dehydration
τ	$(SV)^{-1}$; gm of catalyst hour per mole of feed

APPENDIX I

CALIBRATION OF MICRO-FEEDER

APPENDIX I

CALIBRATION OF MICRO-FEEDER

The micro-feeder was calibrated by feeding sec-butanol at an average room temperature of 72°F. The sec-butanol was collected in a 25 ml Erlenmeyer flask after it has passed through the 1/16 in stainless steel tubing. The Erlenmeyer flask was cooled by ice water in order to prevent the loss of 2-butanol by evaporation. The amount of 2-butanol was obtained by weighing. Prior to the operation of the micro-feeder, the position of the piston in the syringe was set at a level of about 60 cc. The syringe used had a capacity of 100 cc. The results of calibration of micro-feeder is shown in Table A-I-1, and the averages, variances and standard deviations are shown in Table A-I-2.

The mean of feed rate will be estimated as follows (51). The confidence interval of the mean at confidence coefficient α is given by:

$$\bar{x} \pm z_{\alpha/2} (\sigma/\sqrt{n}) \quad (I-1)$$

where \bar{x} is the arithmetic average of sampling variable x_i .

z_{α} is defined by $P(z \geq z_{\alpha}) = \int_{z_{\alpha}}^{\infty} \phi(z)dz = \alpha$

or

$$\Phi(z_{\alpha}) = P(z \leq z_{\alpha}) = 1 - \alpha$$

Table A-I-3 is a list of the most important and commonly used values of z_{α} .

TABLE A-I-1
CALIBRATION OF MICRO-FEEDER

Fluid	sec-butanol				
Feeder	100 cc brass syringe				
Temperature	72°F				
	Velocity of Piston in Syringe				
RUN	10 mm/hr	15 mm/hr	20 mm/hr	30 mm/hr	40 mm/hr
1	6.2600	9.4368	12.5246	18.8406	24.9868
2	6.3036	9.4162	12.5466	18.8588	24.0662
3	6.2822	9.4260	12.5554	18.8284	25.1044
4	6.2698	9.4140	12.5514		25.1016
5	6.2680	9.4446	12.5462		24.9542
Average	6.2767	9.4275	12.5448	18.8426	25.0426

TABLE A-I-2

VARIANCE AND STANDARD DEVIATION OF FEED RATES

Piston Velocity		10 mm/hr	15 mm/hr	20 mm/hr	30 mm/hr	40 mm/hr
Average	μ	6.2767	9.4275	12.5448	18.8426	25.0426
Variance	σ^2	0.000288	0.000172	0.000141	0.000233	0.004695
Standard Deviation	σ	0.01697	0.013114	0.011874	0.015264	0.06852

TABLE A-I-3

SOME PERCENTAGE POINTS OR SIGNIFICANCE POINTS OF THE NORMAL DISTRIBUTION

α	.10	.05	.025	.01	.005
z_{α}	1.282	1.645	1.960	2.326	2.576

n is the sample size

σ is the population standard deviation

σ^2 is the population variance.

Therefore to find the 95% confidence interval for μ (mean) we have

$$1 - \alpha = .95, \alpha/2 = 0.025$$

From Table A-I-3 $z_{\alpha/2} = 1.960$.

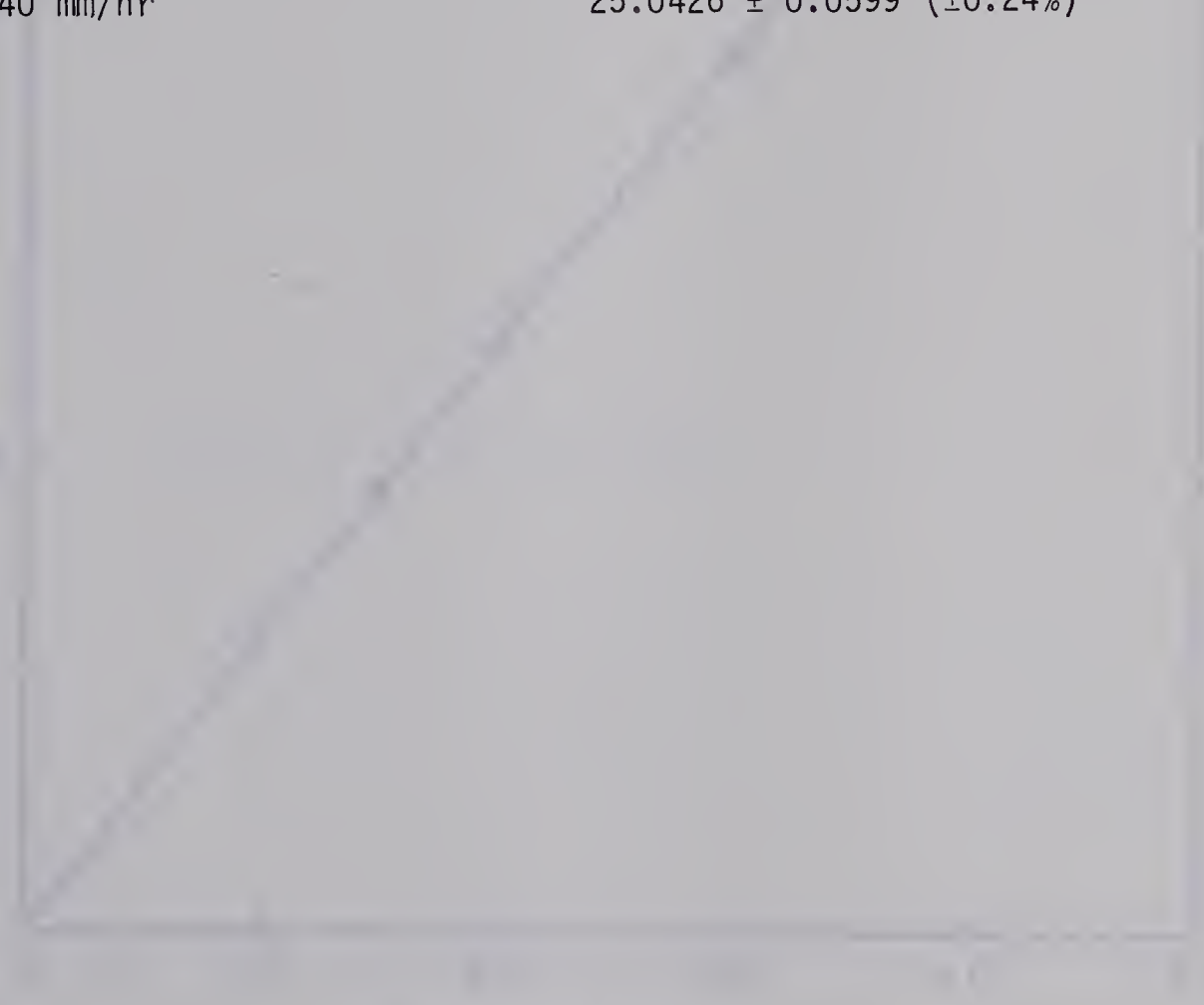
Piston Velocity	10 mm/hr	15 mm/hr	20 mm/hr	30 mm/hr	40 mm/hr
\bar{x}	6.2767	9.4275	12.5448	18.8426	25.0426
\sqrt{n}	2.236	2.236	2.236	1.732	2.236
σ/\sqrt{n}	0.0075	0.0058	0.0052	.0087	0.0306
$z_{\alpha/2}(\sigma/\sqrt{n})$	0.0147	0.0113	0.0101	0.0170	0.0599

Therefore the 95% confidence interval for μ is as given in Table A-I-4.

TABLE A-I-4

MEANS OF FEED RATES OF SEC-BUTANOL

Piston Velocity	Feed rate of sec-Butanol gm/hr
10 mm/hr	6.2767 ± 0.0147 ($\pm 0.23\%$)
15 mm/hr	9.4275 ± 0.0113 ($\pm 0.12\%$)
20 mm/hr	12.5448 ± 0.0101 ($\pm 0.08\%$)
30 mm/hr	18.8426 ± 0.0170 ($\pm 0.10\%$)
40 mm/hr	25.0426 ± 0.0599 ($\pm 0.24\%$)



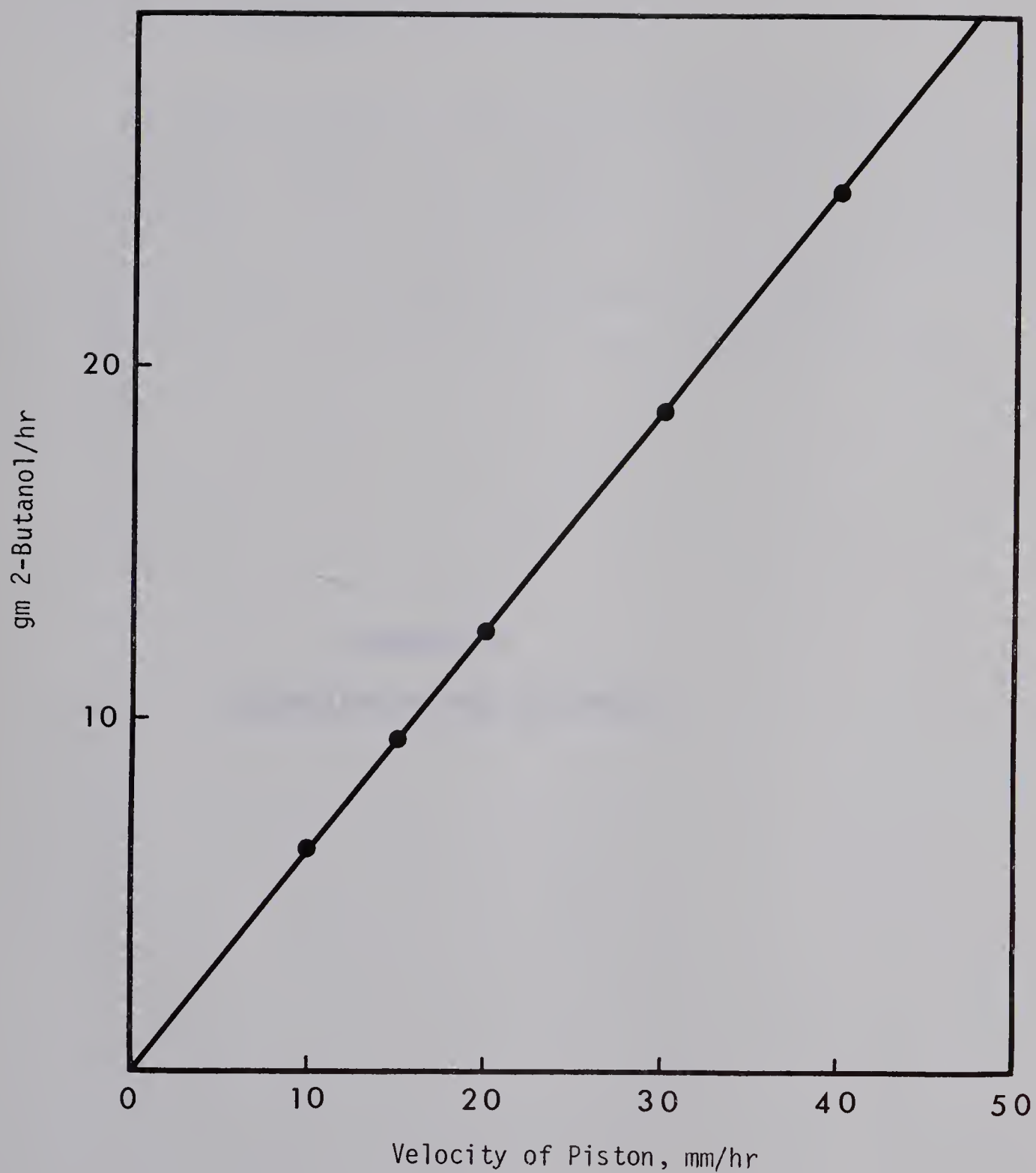


FIGURE A-I-1. CALIBRATION CURVE FOR MICRO FEEDER

APPENDIX II
CALIBRATION OF MASS FLOW METER

APPENDIX II

CALIBRATION OF MASS FLOW METER

The Matheson Mass Flow meter was calibrated by feeding the nitrogen from the cylinder through a regulator controlled at 30 psig, and through a Nullmatic Pressure Regulator where the flow was controlled. The gas flow was read from the mass flow meter and checked by a bubble flow meter. The calibration is as shown in Table A-II-1 and Figure A-II-1.

TABLE A-II-1

CALIBRATION CURVE APPROXIMATION (LINEAR LEAST
SQUARES) FOR MATHESON FLOW METER

X = READING.

Y = CC/MIN AT 21°C & 760 MMHG.

THE COEFFICIENTS OF THE POLYNOMIAL ARE,

A0 = 0.20043

A1 = 0.94470

A2 = -0.00231

REGENERATED DATA

X MEASURED	Y OBSERVED	Y CALCULATED	PCT ERROR
19.60000	17.78000	17.82700	0.26434
17.60000	16.17000	16.10988	0.37177
16.60000	15.29000	15.24437	0.29837
15.00000	13.88000	13.84993	0.21659
12.60000	11.60000	11.73604	1.17277
10.00000	9.38000	9.41588	0.38254
6.50000	6.38000	6.24315	2.14485
3.00000	2.96000	3.01369	1.81410

VARIANCE = 0.007173

STANDARD DEVIATION = 0.084694

MAXIMUM PCT ERROR = 2.144855

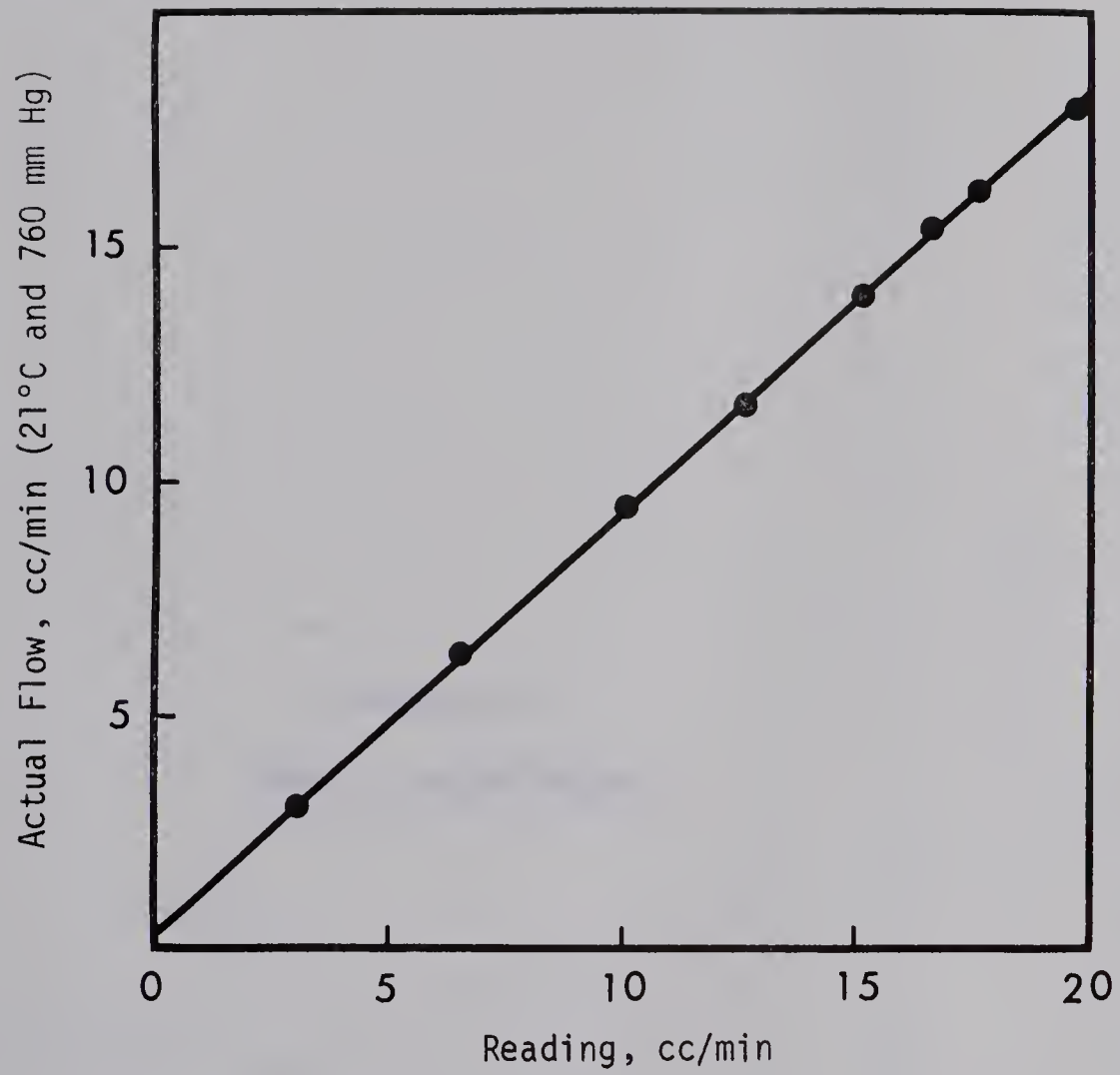


FIGURE A-II-1. CALIBRATION CURVE FOR MATHESON MASS FLOW METER

APPENDIX III
SAMPLE CHROMATOGRAMS

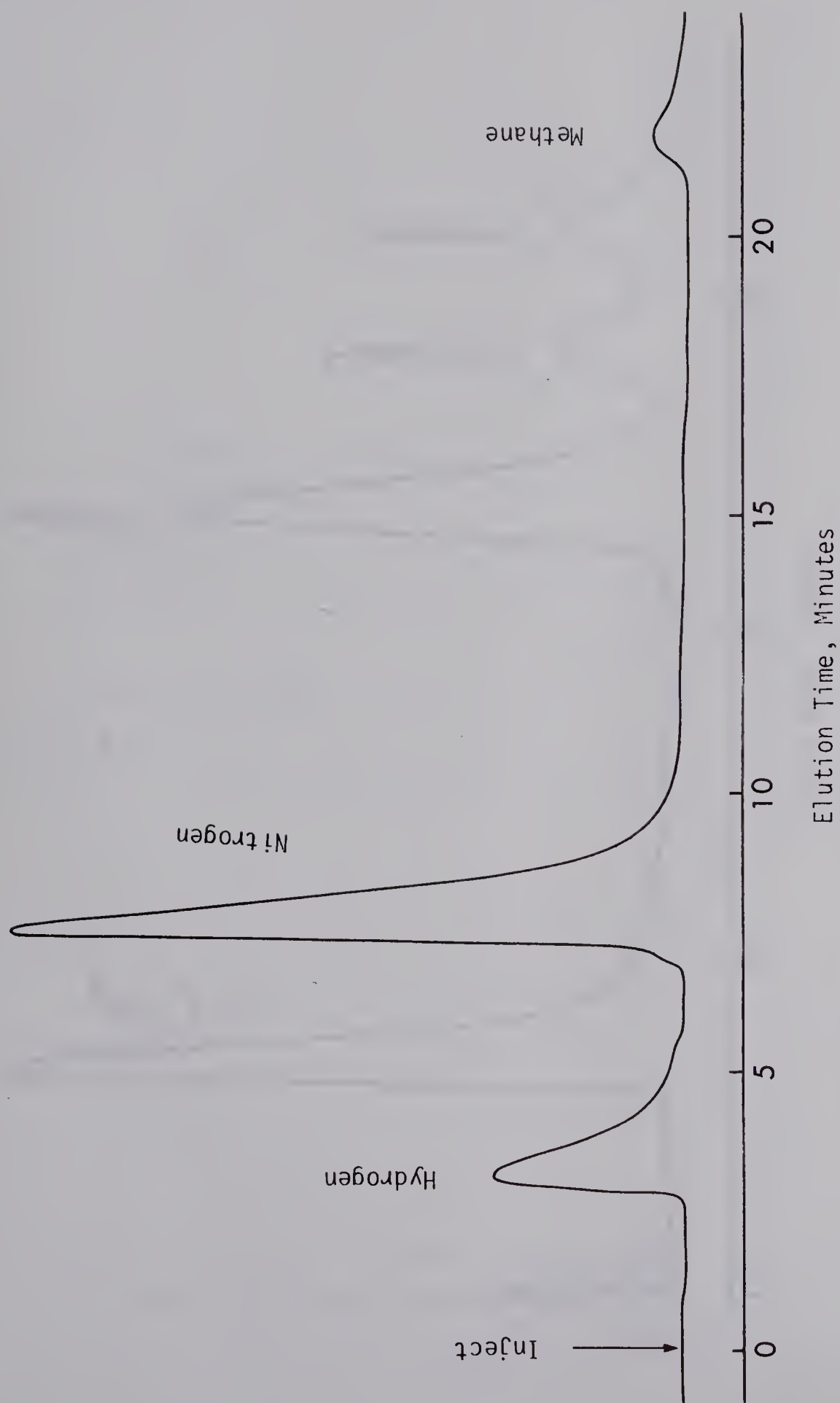


FIGURE A-III-1. CHROMATOGRAM FOR GAS ANALYSIS CHARCOAL COLUMN

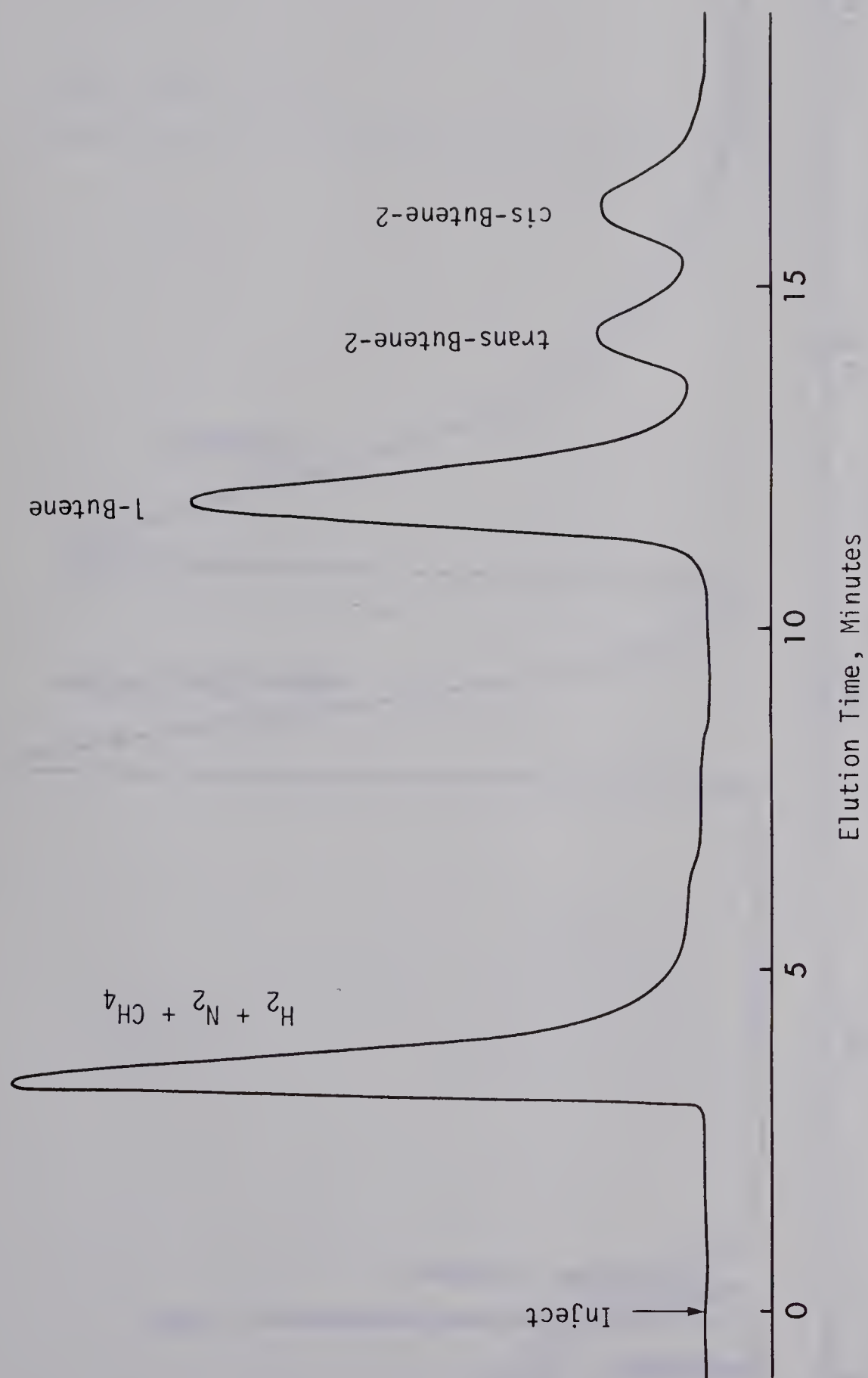


FIGURE A-III-2. CHROMATOGRAM FOR GAS ANALYSIS UCON ON CELITE COLUMN

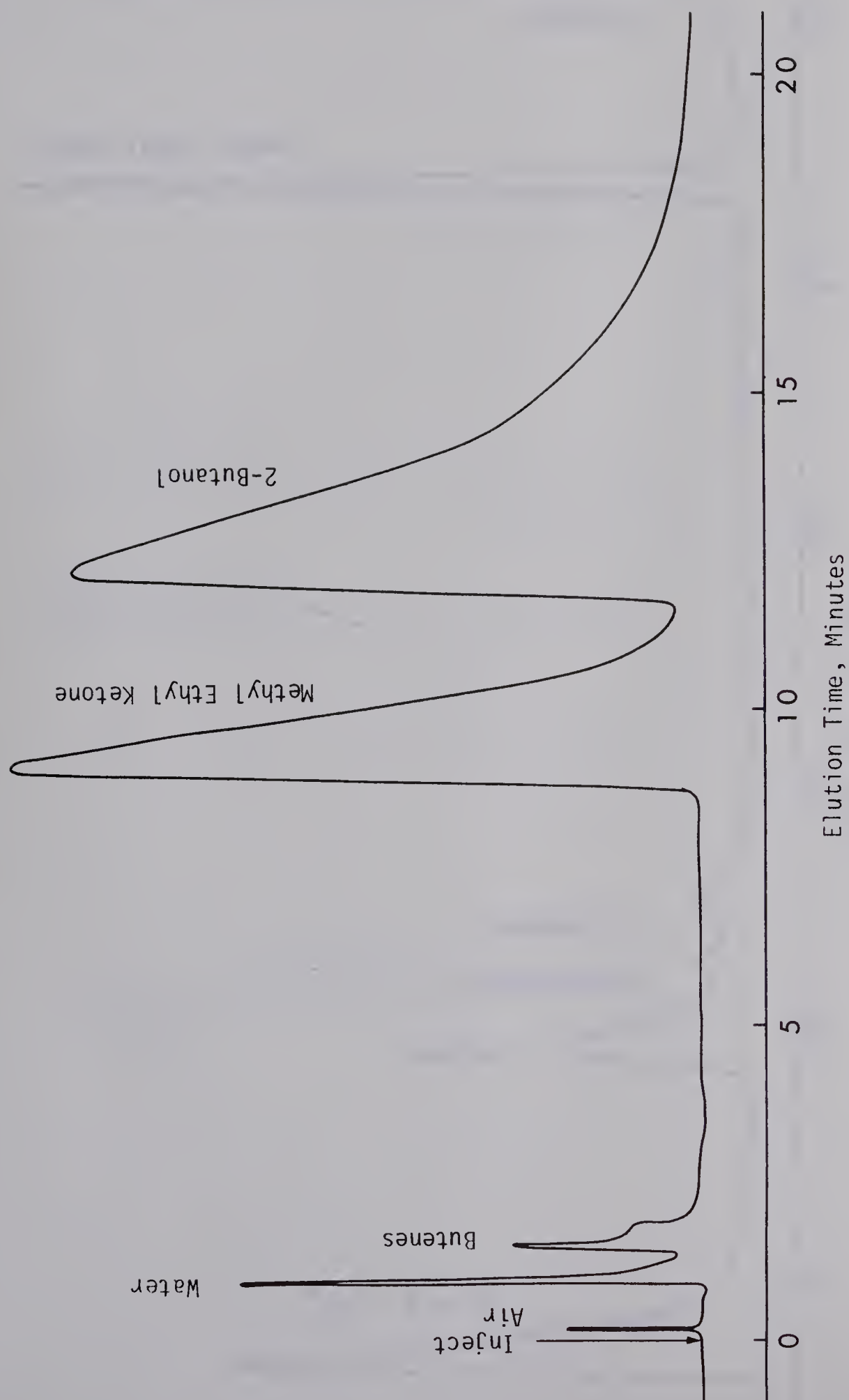


FIGURE A-III-3. CHROMATOGRAM FOR LIQUID ANALYSIS PORAPAK COLUMN

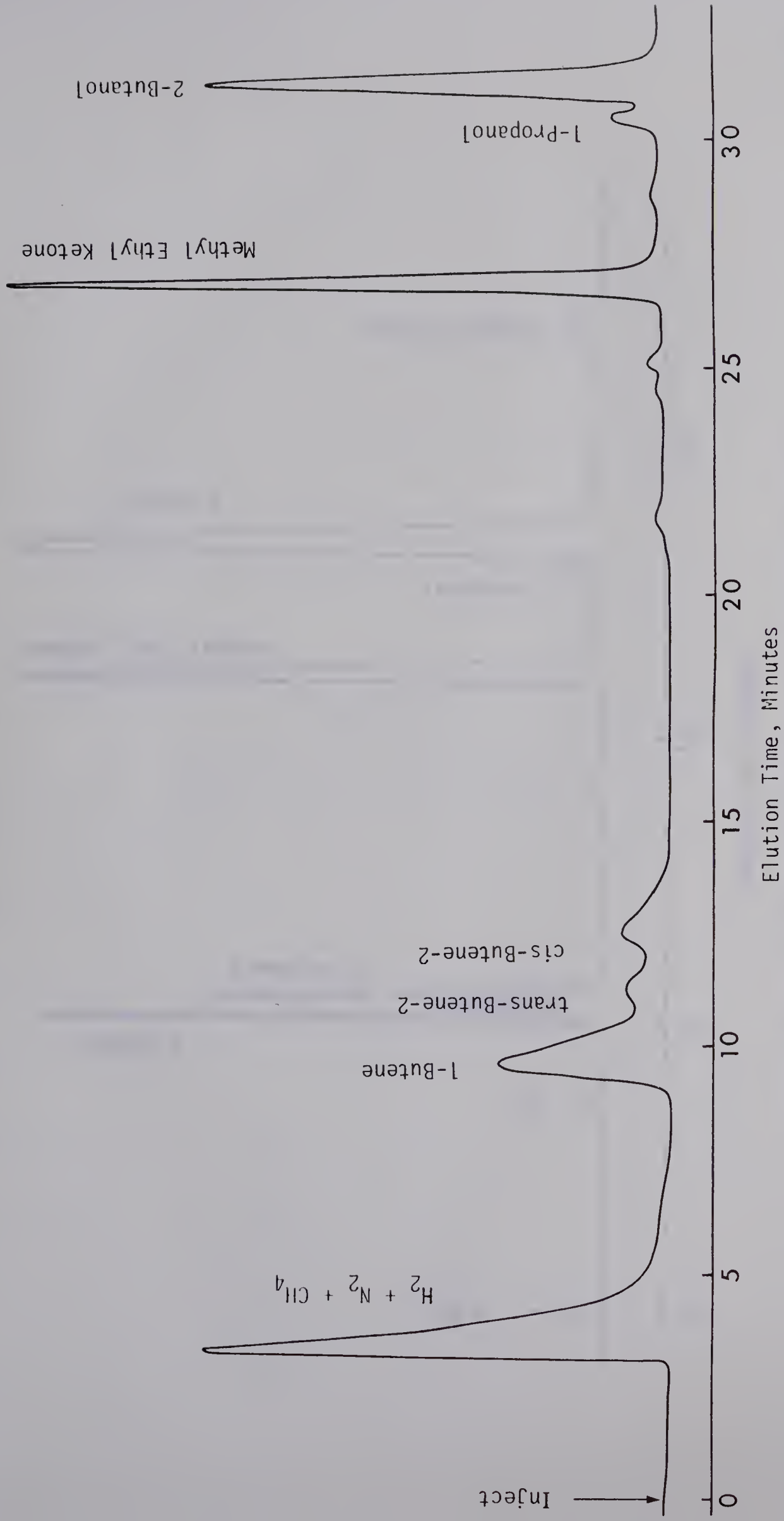


FIGURE A-III-4. CHROMATOGRAM FOR VAPOUR PRODUCT ANALYSIS UCON ON CELITE COLUMN

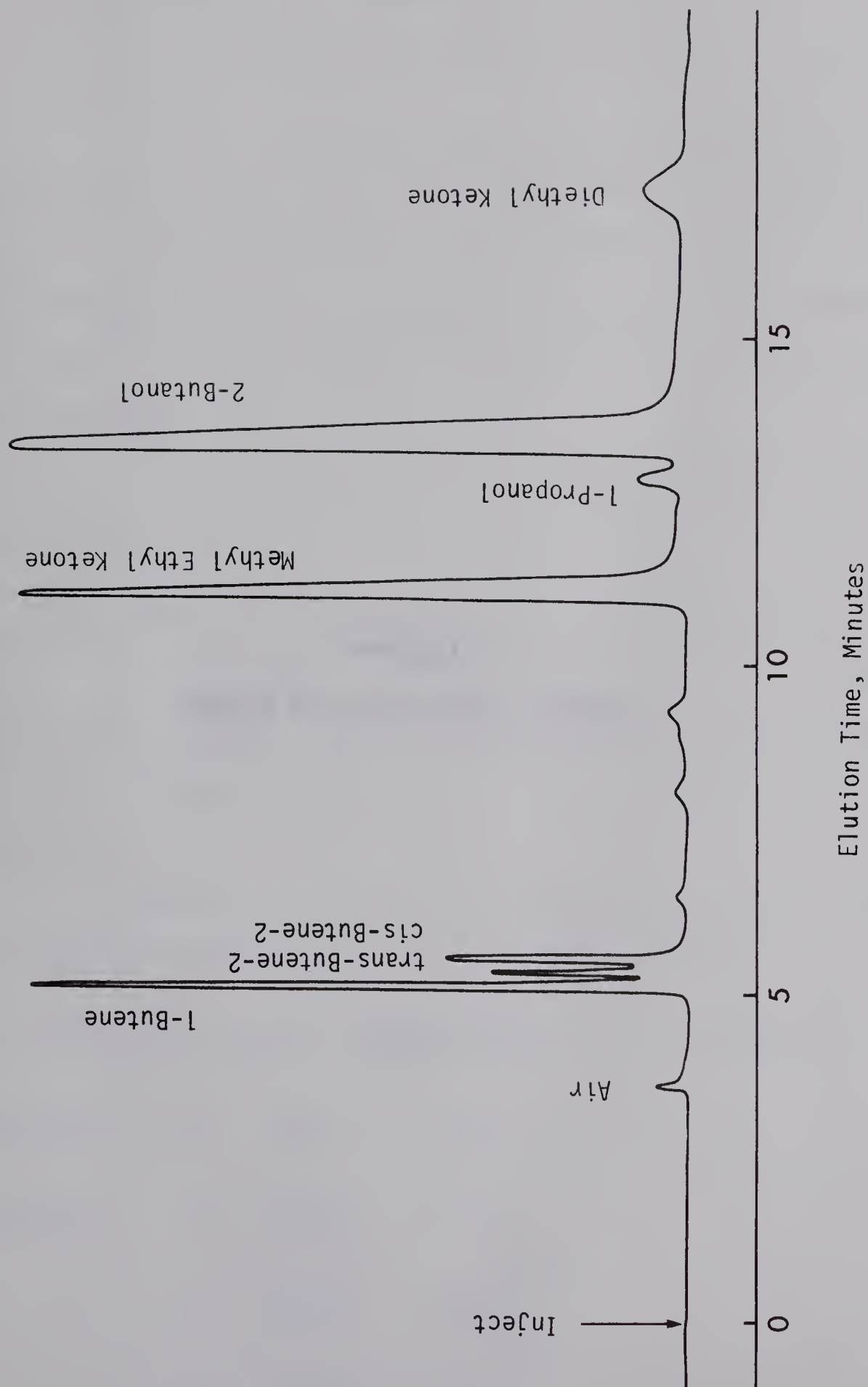


FIGURE A-III-5. CHROMATOGRAM FOR LIQUID ANALYSIS UCON ON CELITE COLUMN

1. The first step is to determine the

total number of observations.

2. The second step is to calculate the

mean of the observations.

3. The third step is to calculate the

variance of the observations.

4. The fourth step is to calculate the

standard deviation of the observations.

5. The fifth step is to calculate the

coefficient of variation of the observations.

APPENDIX IV

METHOD OF CALCULATION OF RESULTS

1. The first step is to determine the

total number of observations.

2. The second step is to calculate the

mean of the observations.

3. The third step is to calculate the

variance of the observations.

4. The fourth step is to calculate the

standard deviation of the observations.

5. The fifth step is to calculate the

coefficient of variation of the observations.

6. The sixth step is to calculate the

mean square error of the observations.

APPENDIX IV

METHOD OF CALCULATION OF RESULTS

For each run the experimental conditions were first determined before calculation was made. Room temperature, atmospheric pressure, reaction temperature, reaction pressure, weight of catalyst, nitrogen feed rate, sec-butanol feed rate, space velocity, (space velocity)⁻¹, fractional change in volume and initial concentration were determined.

For each product sample, two separate methods of calculation were carried out.

1. Calculation for coupled reactor gas chromatograph system

For each sample, calculations are carried out for mole percent of each component, overall material balance, carbon, hydrogen and oxygen balances, 2-butanol conversion and conversion by dehydrogenation and dehydration.

A sample calculation is given below for run no. 24. The experimental conditions determined are given in Appendix V.

For the charcoal column, ($\frac{\text{component area}}{\text{total area}}$) were calculated.

Peak areas are $H_2 = 3944$, $N_2 = 463724$, $CH_4 = 273$.

$$\text{Therefore } H_2 = \frac{3944}{467641} = 0.0084$$

$$N_2 = \frac{463424}{467641} = 0.9909$$

$$CH_4 = \frac{273}{467641} = 0.0005$$

On the Ucon column for gases again ($\frac{\text{component area}}{\text{total area}}$) were calculated.

Peak 1 on this column corresponds to all the three gases analyzed on the charcoal column.

Peak areas are ($\text{H}_2 + \text{N}_2 + \text{CH}_4$) = 552228, n-C_4 = 5965, $\text{t-C}_4 = \text{c-C}_4 = 0.0$.

$$\text{Thus } \text{H}_2 = (0.0084 \times 552228)/558193 = .0083$$

$$\text{N}_2 = (0.9909 \times 552228)/558193 = .9803$$

$$\text{CH}_4 = (0.0005 \times 552228)/558193 = .0004$$

$$\text{n-C}_4 = 5965/558193 = .0106$$

$$\text{t-C}_4 = - = -$$

$$\text{c-C}_4 = - = -$$

The ratio ($\frac{\text{water area}}{\text{sec-butanol}}$) was then calculated for the Porapak column.

$$(\text{H}_2\text{O})_p = 618/271750 = .0022$$

Area percent in the main Ucon column was then determined.

$$\text{Water area in Ucon column} = .0022 \times 1417627 = 3119$$

Peak areas are ($\text{H}_2 + \text{N}_2 + \text{CH}_4 + \text{nC}_4$) = 207415, MEK = 184160, 2-butanol = 1417627, DEK = 1742.

Thus

$$\text{H}_2 = (.0083 \times 207415) \times \frac{100.0}{1814063} = .095$$

$$\text{N}_2 = (.9803 \times 207415) \times \frac{100.0}{1814063} = 11.208$$

$$\text{CH}_4 = (.0004 \times 207415) \times \frac{100.0}{1814063} = .006$$

$$\text{n-C}_4 = (.0106 \times 207415) \times \frac{100.0}{1814063} = .121$$

$$t-C_4 = \quad - \quad = \quad -$$

$$c-C_4 = \quad - \quad = \quad -$$

$$MEK = 184160 \times \frac{100.0}{1814063} = 10.151$$

$$2-BuOH = 1417627 \times \frac{100.0}{1814063} = 78.142$$

$$DEK = 1742 \times \frac{100.0}{1814063} = 0.096$$

$$H_2O = 3119 \times \frac{100.0}{1814063} = 0.177$$

These area percentages are as shown in Appendix V together with weight and mole percentages which were calculated by the following.

$$\text{Component wt. \%} = \left(\frac{100}{\text{total wt.}} \right) \times \text{area \%} \times \text{Relative Response Factor}$$

$$\text{Component mol \%} = \frac{\text{component wt. \%}}{\text{molecular wt.}} \times \frac{100}{\text{total moles}}$$

To determine the material balance, the weight of each component was calculated. Knowing the mole percent of N_2 in the product and exact mole in feed,

$$\text{Wt. of component} = \text{Mol. \%} \times \text{molecular weight} \times \frac{\text{moles of } N_2 \text{ in feed}}{N_2 \text{ mole \% in product}}$$

Therefore,

Component	Weight	Moles
H_2	.04492	.02228
CH_4	.00055	.00003
$1-C_4$.01590	.00028
$t-C_4$	-	-

c-C ₄	-	-
MEK	1.38878	.01926
2-BuOH	10.90320	.14710
DEK	0.01398	.00016
H ₂ O	<u>0.018026</u>	.00100
Total	12.38535	

Using equations as defined in Section 5.1:

$$\text{Material balance} = \frac{12.38535}{12.54484} \times 100 = 98.7\%$$

$$\begin{aligned} \text{Carbon balance} &= \frac{4(.00028 + .01926 + .1471) + 1(.00003) + 5(.00016)}{4(.16925)} \times 100 \\ &= 98.6\% \end{aligned}$$

Similarly hydrogen and oxygen balances were calculated and shown in Appendix V.

Conversion calculations:

$$\text{2-butanol conversion} = \left(1 - \frac{.14710}{.16925}\right) = .13047$$

$$\text{conversion (dehydrogenation)} = \frac{.01926}{.16925} = .11386$$

$$\text{conversion (dehydration)} = \frac{.00028}{.16925} = .00167$$

2. Calculation for conventional system

Weight and mole of components in liquid product were first determined.

Peak areas are n-C₄ = 269, unk = 6, MEK = 40776, PrOH = 150, 2-butanol = 349038, DEK = 1.

$$\text{Water area in Ucon column} = .0022 \times 349038 = 768$$

$$\text{Wt. of component} = \frac{\text{chromatogram area}}{\text{area}} \times \frac{\text{relative response factor}}{\text{factor}} \times \frac{\text{wt of liquid product}}{\text{total weight}}$$

$$\therefore \text{MEK} = 40776 \times .94 \times \frac{12.3030}{373871} = 1.26104$$

Component	Weight	Moles
1-C ₄	.00791	.00014
t-C ₄	-	-
c-C ₄	-	-
ukn	.00014	.000003
H ₂ O	.01761	.000978
MEK	1.26104	.01749
PrOH	.00454	.00008
2-BuOH	11.00909	.14853
DEK	.00003	<u>.00000</u>
Total		.16722

Moles of components in the gas product were then determined.

$$\text{Total moles of gas (wet test meter)} = (.0776 \times 1.0025 \times \frac{28317}{22414}) \times (\frac{700}{760}) \times (\frac{273}{296}) = .08349$$

$$\text{moles of component} = \left\{ \left(\frac{\text{area}}{\text{ratio}} \times \frac{\text{relative response}}{\text{factor}} \right) / \frac{\text{molecular weight}}{\text{weight}} \right\} \times \frac{.08349}{.04113}$$

Thus

Component	Moles
H ₂	.02524
N ₂	.05788
CH ₄	.00003
1-C ₄	.00034
t-C ₄	-
c-C ₄	<u>-</u>
	.08349

$$\therefore \text{Total mol (gas + liquid)} = (.08349 + .16722) = 0.25071$$

$$\text{mol \% of component} = \text{mol of component} \times \frac{100}{\text{total mol}}$$

Thus

Component	Mol %
H ₂	10.10
N ₂	23.05
CH ₄	0.02
1-C ₄	0.19
t-C ₄	-
c-C ₄	-
ukn	-
H ₂ O	.40
MEK	6.97
PrOH	0.03
2-BuOH	59.23
DEK	-

These results as well as (mole/mol 2-butanol fed) are as shown in Appendix V.

$$\text{Material balance} = \frac{0.08349 + 12.3030}{12.54484 + (.04747 \times 28.016)} \times 100 = 94.68$$

Carbon, hydrogen, oxygen balances and conversions are calculated as above and as shown in Appendix V.

The computer program that was used for the calculation of the results is presented in Appendix VII.

APPENDIX V
EXPERIMENTAL RESULTS

RUN NUMBER 1

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.0	DEG. CENTG.
ATMOPHERIC PRESSURE	701.6	MM HG.
REACTION TEMPERATURE	385.0	DEG. CENTG.
REACTION PRESSURE	704.6	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.11683	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.71003	
INITIAL CONCENTRATION	0.02255	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	72.0	DEG. CELSIUS
ATMOSPHERIC PRESSURE	701.6	MM. HG.
REACTION TEMPERATURE	382.0	DEG. CELSIUS
REACTION PRESSURE	704.6	MM. HG.
WT. OF CATALYST	6.8200	GRAMS
NITROGEN FEED	0.11683	G. MOL/VOL
2-BUTANOL FEED	0.16922	G. MOL/VOL
SPACE VELOCITY	0.02472	MOL/VOL-HR.
12.4.	40.44303	L. HR./VOL.
VOLUME CHANGE	0.11003	
INITIAL CONCENTRATION	0.02222	MOL/VOL-LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	24.013661	21.244019	33.561746
HYDROGEN	0.250315	0.820569	18.015182
METHANE	0.008423	0.005211	0.014379
BUTENE-1	0.887211	0.860965	0.679212
TRANS-BUTENE-2	0.107593	0.098570	0.077762
CIS-BUTENE-2	0.092636	0.082957	0.065444
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	26.614117	27.155676	16.670143
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	47.159618	49.076514	29.305711
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.866421	0.655515	1.610416
TOTAL	99.999999	99.999999	100.000000

MATERIAL BALANCE	96.727746	PERCENT
CARBON BALANCE	96.261398	PERCENT
HYDROGEN BALANCE	97.143274	PERCENT
OXYGEN BALANCE	97.874745	PERCENT

2-BUTANOL CONVERSION 0.39724
 CONV. TO 1. KETONE 0.34286 2. BUTENES 0.01691

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	32.007696	
HYDROGEN	17.181004	0.337507
METHANE	0.013713	0.000269
BUTENE-1	0.811363	0.015938
TRANS BUTENE-2	0.115251	0.002264
CIS BUTENE-2	0.112043	0.002201
UNKNOWN-1	0.002300	0.000045
METHYL ETHYL KETONE	16.573436	0.325572
1-PROPANOL	0.006128	0.000120
SEC-BUTANOL	31.447981	0.617771
DIETHYL KETONE	0.000941	0.000018
WATER	1.728139	0.033948
TOTAL	100.000000	

MATERIAL BALANCE	95.571614	PERCENT
CARBON BALANCE	96.392913	PERCENT
HYDROGEN BALANCE	96.906684	PERCENT
OXYGEN BALANCE	97.743159	PERCENT

2-BUTANOL CONVERSION 0.38222
 CONV. TO 1. KETONE 0.32557 2. BUTENES 0.02040

COMPARISON OF MATERIAL BALANCE

COMPONENT	AS RECORDED	AS RECORDED	AS RECORDED
ETHANOL	24.0000	24.0000	24.0000
ETHANOL-1	0.0000	0.0000	0.0000
ETHANOL-2	0.0000	0.0000	0.0000
BUTANE-1	0.0000	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	24.0000	24.0000	24.0000
1-PROPANOL	0.0000	0.0000	0.0000
SEC-BUTANOL	44.0000	44.0000	44.0000
DI-ETHYL KETONE	0.0000	0.0000	0.0000
WATER	0.0000	0.0000	0.0000
TOTAL	96.0000	96.0000	96.0000
OXYGEN BALANCE	97.8750	97.8750	97.8750
HYDROGEN BALANCE	97.1437	97.1437	97.1437
CARBON BALANCE	96.2613	96.2613	96.2613
MATERIAL BALANCE	96.2776	96.2776	96.2776
CONV. TO 1. KETONE 0.2458	0.2458	0.2458	0.2458
2-BUTANOL CONVERSION	0.3825	0.3825	0.3825

COMPARISON OF SYSTEM

COMMENT	WOLF PERCENT	WOLF PERCENT
NITROGEN	32.0000	32.0000
HYDROGEN	17.1604	17.1604
METHANE	0.0137	0.0137
BUTANE-1	0.0136	0.0136
TRANS BUTENE-2	0.1125	0.1125
CIS BUTENE-2	0.1120	0.1120
UNKNOWN-1	0.0030	0.0030
METHYL ETHYL KETONE	16.2345	16.2345
1-PROPANOL	0.0012	0.0012
SEC-BUTANOL	31.4481	31.4481
DIETHYL KETONE	0.0000	0.0000
WATER	1.2581	1.2581
TOTAL	100.0000	100.0000
OXYGEN BALANCE	97.8750	97.8750
HYDROGEN BALANCE	97.1437	97.1437
CARBON BALANCE	96.2613	96.2613
MATERIAL BALANCE	96.2776	96.2776
CONV. TO 1. KETONE 0.2458	0.2458	0.2458
2-BUTANOL CONVERSION	0.3825	0.3825

RUN NUMBER 2

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.8	DEG. CENTG.
ATMOPHERIC PRESSURE	706.1	MM HG.
REACTION TEMPERATURE	350.9	DEG. CENTG.
REACTION PRESSURE	708.1	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.07705	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.76169	
INITIAL CONCENTRATION	0.02619	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	27.8	DEG. C.
ATMOSPHERIC PRESSURE	700.1	MM. HG.
REACTION TEMPERATURE	250.9	DEG. C.
REACTION PRESSURE	708.1	MM. HG.
MT. OF CATALYST	6.8450	GRAM.
NITROGEN FEED	0.0750	G. MIN.
2-NUTROL FEED	0.1625	G. MIN.
SPACE VELOCITY	0.02475	MIN. PER G.
LVS.V.	0.00303	G. PER L.
VOLUME CHANGE	0.7618	
INITIAL CONCENTRATION	0.05819	MOLES PER L.

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	17.168354	15.005765	29.812594
HYDROGEN	0.062149	0.201288	5.557462
METHANE	0.000000	0.000000	0.000000
BUTENE-1	0.166693	0.159819	0.158556
TRANS-BUTENE-2	0.013121	0.011876	0.011782
CIS-BUTENE-2	0.019088	0.016888	0.016755
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	8.665913	8.736029	6.744140
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	73.489808	75.558220	56.740618
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.414870	0.310110	0.958090

TOTAL	099.999999	100.000000	100.000000
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MATERIAL BALANCE	97.476377	PERCENT
CARBON BALANCE	97.240024	PERCENT
HYDROGEN BALANCE	97.113058	PERCENT
OXYGEN BALANCE	98.417494	PERCENT

2-BUTANOL CONVERSION 0.13345
 CONV. TO 1. KETONE 0.10299 2. BUTENES 0.00285

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	28.677664	
HYDROGEN	5.345896	0.080959
METHANE	0.000000	0.000000
BUTENE-1	0.213606	0.003234
TRANS BUTENE-2	0.022217	0.000336
CIS BUTENE-2	0.035938	0.000544
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	6.702886	0.101510
1-PROPANOL	0.005963	0.000090
SEC-BUTANOL	57.984503	0.878132
DIETHYL KETONE	0.032229	0.000488
WATER	0.979093	0.014827

TOTAL	99.999999
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MATERIAL BALANCE	98.157925	PERCENT
CARBON BALANCE	98.443593	PERCENT
HYDROGEN BALANCE	98.235070	PERCENT
OXYGEN BALANCE	99.504848	PERCENT

2-BUTANOL CONVERSION 0.12186
 CONV. TO 1. KETONE 0.10151 2. BUTENES 0.00411

COMPARISON OF THE TWO SYSTEMS

COMPONENT	PERCENT	PERCENT	PERCENT
WATER	0.41410	0.31010	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-2-PENTENE-2	0.01000	0.01000	0.00000
TRANS-2-PENTENE-2	0.01000	0.01000	0.00000
BUTENE-1	0.01000	0.01000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	0.00000	0.00000	0.00000

OXYGEN BALANCE 97.4134%
 HYDROGEN BALANCE 97.1130%
 CARBON BALANCE 97.2400%
 MATERIAL BALANCE 97.4747%

CONV. TO 1. KETONE 0.1020% 2. BUTENE 0.0020%
 3-BUTANOL CONVERSION 0.1344%

COMPARISON OF THE TWO SYSTEMS

COMPONENT	PERCENT	PERCENT	PERCENT
WATER	0.41410	0.31010	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-2-PENTENE-2	0.01000	0.01000	0.00000
TRANS-2-PENTENE-2	0.01000	0.01000	0.00000
BUTENE-1	0.01000	0.01000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	0.00000	0.00000	0.00000

OXYGEN BALANCE 97.4134%
 HYDROGEN BALANCE 97.1130%
 CARBON BALANCE 97.2400%
 MATERIAL BALANCE 97.4747%

CONV. TO 1. KETONE 0.1020% 2. BUTENE 0.0020%
 3-BUTANOL CONVERSION 0.1344%

RUN NUMBER 3

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	24.0	DEG. CENTG.
ATMOPHERIC PRESSURE	701.4	MM HG.
REACTION TEMPERATURE	391.8	DEG. CENTG.
REACTION PRESSURE	705.4	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.02485	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.88647	
INITIAL CONCENTRATION	0.03300	MOLES/LITER

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EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.0 DEG. CELSIUS
ATMOSPHERIC PRESSURE	761.4 MM. HG.
REACTION TEMPERATURE	301.4 DEG. CELSIUS
REACTION PRESSURE	762.4 MM. HG.
WT. OF CATALYST	0.8450 GRAMS
NITROGEN FEED	0.0245 G. MINUTE
2-BUTANOL FEED	0.1625 G. MINUTE
SPACE VELOCITY	0.0245 MINUTE PER GRAM
15.5.	0.4307 G. MINUTE PER GRAM
VOLUME CHANGE	0.8847
INITIAL CONCENTRATION	0.0330 MOLES PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	6.088599	5.264091	10.222514
HYDROGEN	0.202364	0.648318	17.495994
METHANE	0.031776	0.019214	0.065164
BUTENE-1	0.733703	0.695835	0.674766
TRANS-BUTENE-2	0.121534	0.108815	0.105520
CIS-BUTENE-2	0.108008	0.094527	0.091665
UNKNOWN-1	0.010853	0.008289	0.009804
METHYL ETHYL KETONE	38.669820	38.561013	29.097359
1-PROPANOL	0.071645	0.069923	0.063298
SEC-BUTANOL	52.589039	53.484310	39.258291
DI-ETHYL KETONE	0.095553	0.101366	0.064022
WATER	1.277101	0.944292	2.851599
TOTAL	099.999999	099.999999	100.000000

MATERIAL BALANCE	99.907372	PERCENT
CARBON BALANCE	99.668597	PERCENT
HYDROGEN BALANCE	96.899413	PERCENT
OXYGEN BALANCE	102.489168	PERCENT

2-BUTANOL CONVERSION 0.43596
 CONV. TO 1. KETONE 0.41805 2. BUTENES 0.01252

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	14.932083	
HYDROGEN	25.556494	0.434873
METHANE	0.095186	0.001619
BUTENE-1	1.352112	0.023007
TRANS BUTENE-2	0.257252	0.004377
CIS BUTENE-2	0.258263	0.004394
UNKNOWN-1	0.013874	0.000236
METHYL ETHYL KETONE	22.528160	0.383342
1-PROPANOL	0.050281	0.000855
SEC-BUTANOL	32.574334	0.554289
DIETHYL KETONE	0.015858	0.000269
WATER	2.366097	0.040261
TOTAL	099.999999	

MATERIAL BALANCE	101.407266	PERCENT
CARBON BALANCE	97.079588	PERCENT
HYDROGEN BALANCE	98.301668	PERCENT
OXYGEN BALANCE	97.901943	PERCENT

2-BUTANOL CONVERSION 0.44571
 CONV. TO 1. KETONE 0.38334 2. BUTENES 0.03177

COMPARISON OF THEORETICAL AND ACTUAL COMPOSITION

THEORETICAL COMPOSITION		ACTUAL COMPOSITION		PERCENT DIFFERENCE	
WATER	1.2710	1.2710	0.0000	0.0000	0.0000
DIETHYL KETONE	0.0000	0.0000	0.0000	0.0000	0.0000
SEC-BUTANOL	0.0000	0.0000	0.0000	0.0000	0.0000
1-PROPANOL	0.0000	0.0000	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	0.0000	0.0000	0.0000	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000	0.0000	0.0000
BUTENE-1	0.0000	0.0000	0.0000	0.0000	0.0000
METHANE	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000
NITROGEN	0.0000	0.0000	0.0000	0.0000	0.0000
TOTAL		0.0000	0.0000	0.0000	0.0000
OXYGEN BALANCE		102.4818	PERCENT		
HYDROGEN BALANCE		84.8012	PERCENT		
CARBON BALANCE		89.6882	PERCENT		
MATERIAL BALANCE		98.9032	PERCENT		
CONV. TO 1. KETONE 0.4186 2. BUTENE 0.0152 2-BUTANOL CONVERSION 0.4324					

COMPOSITIONAL SYSTEM

COMPOSITIONAL SYSTEM		PERCENT DIFFERENCE		THEORETICAL COMPOSITION	
WATER	2.1600	2.1600	0.0000	0.0000	0.0000
DIETHYL KETONE	0.0000	0.0000	0.0000	0.0000	0.0000
SEC-BUTANOL	0.0000	0.0000	0.0000	0.0000	0.0000
1-PROPANOL	0.0000	0.0000	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	0.0000	0.0000	0.0000	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000	0.0000	0.0000
BUTENE-1	0.0000	0.0000	0.0000	0.0000	0.0000
METHANE	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000
NITROGEN	0.0000	0.0000	0.0000	0.0000	0.0000
TOTAL		0.0000	0.0000	0.0000	0.0000
OXYGEN BALANCE		102.4818	PERCENT		
HYDROGEN BALANCE		84.8012	PERCENT		
CARBON BALANCE		89.6882	PERCENT		
MATERIAL BALANCE		98.9032	PERCENT		
CONV. TO 1. KETONE 0.4186 2. BUTENE 0.0152 2-BUTANOL CONVERSION 0.4324					

RUN NUMBER 4

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	701.6	MM HG.
REACTION TEMPERATURE	394.0	DEG. CENTG.
REACTION PRESSURE	704.6	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.04225	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.83347	
INITIAL CONCENTRATION	0.03039	MOLES/LITER

EXPERIMENTAL CONDITIONS

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.0	SEC. LITG.
ATMOSPHERIC PRESSURE	701.6	MM HG.
REACTION TEMPERATURE	394.0	SEC. LITG.
REACTION PRESSURE	704.6	MM HG.
WT. OF CATALYST	0.0450	GRAM.
NITROGEN FEED	0.0455	CC. MIN.
2-BUTANOL FEED	0.1925	CC. MIN.
SPACE VELOCITY	0.0245	MIN. LITG.
INSTR.	0.0430	MIN. LITG.
VOLUME CHANGE	0.0334	
INITIAL CONCENTRATION	0.0303	MOLES LITG.

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.256706	8.896734	14.480000
HYDROGEN	0.375296	1.206274	27.283470
METHANE	0.055616	0.033739	0.095902
BUTENE-1	1.418088	1.349292	1.096620
TRANS-BUTENE-2	0.252467	0.226784	0.184315
CIS-BUTENE-2	0.214146	0.188031	0.152819
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	37.258670	37.275223	23.573772
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	48.855449	49.849498	30.666871
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	1.313558	0.974422	2.466226
TOTAL	099.999999	100.000000	099.999999

MATERIAL BALANCE	96.640380	PERCENT
CARBON BALANCE	96.041411	PERCENT
HYDROGEN BALANCE	97.701612	PERCENT
OXYGEN BALANCE	97.780372	PERCENT

2-BUTANOL CONVERSION 0.47120
 CONV. TO 1. KETONE 0.40648 2. BUTENES 0.02472

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	13.054060	
HYDROGEN	24.596690	0.399916
METHANE	0.086458	0.001405
BUTENE-1	1.377957	0.022404
TRANS BUTENE-2	0.271501	0.004414
CIS BUTENE-2	0.252572	0.004106
UNKNOWN-1	0.004682	0.000076
METHYL ETHYL KETONE	24.222742	0.393836
1-PROPANOL	0.036856	0.000599
SEC-BUTANOL	33.409598	0.543205
DIETHYL KETONE	0.000082	0.000001
WATER	2.686796	0.043684
TOTAL	100.000000	

MATERIAL BALANCE	96.148694	PERCENT
CARBON BALANCE	96.876951	PERCENT
HYDROGEN BALANCE	97.277789	PERCENT
OXYGEN BALANCE	98.132701	PERCENT

2-BUTANOL CONVERSION 0.45679
 CONV. TO 1. KETONE 0.39383 2. BUTENES 0.03092

COMBUSTION BALANCE SHEET

COMBUSTION		FUEL		AIR		TOTAL	
WATER	1.31358	0.00000	0.00000	0.00000	0.00000	1.31358	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
SEC-BUTANOL	44.85249	0.00000	0.00000	0.00000	0.00000	44.85249	0.00000
I-PROPANOL	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	37.25870	0.00000	0.00000	0.00000	0.00000	37.25870	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.21415	0.00000	0.00000	0.00000	0.00000	0.21415	0.00000
TRANS-BUTENE-2	1.25273	0.00000	0.00000	0.00000	0.00000	1.25273	0.00000
BUTENE-1	1.31358	0.00000	0.00000	0.00000	0.00000	1.31358	0.00000
METHANE	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HYDROGEN	0.17501	0.00000	0.00000	0.00000	0.00000	0.17501	0.00000
NITROGEN	10.25000	0.00000	0.00000	0.00000	0.00000	10.25000	0.00000

OXYGEN BALANCE 97.23388 PERCENT
HYDROGEN BALANCE 11.70115 PERCENT
CARBON BALANCE 64.61411 PERCENT
MATERIAL BALANCE 99.84030 PERCENT

2-BUTANOL COMBUSTION
CONV. TO 1. KETONE 0.00000
2. BUTENES 0.00000

COMBUSTION BALANCE SHEET

COMBUSTION		FUEL		AIR		TOTAL	
WATER	5.45639	0.00000	0.00000	0.00000	0.00000	5.45639	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
SEC-BUTANOL	37.25870	0.00000	0.00000	0.00000	0.00000	37.25870	0.00000
I-PROPANOL	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	34.25242	0.00000	0.00000	0.00000	0.00000	34.25242	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.25273	0.00000	0.00000	0.00000	0.00000	0.25273	0.00000
TRANS-BUTENE-2	0.21415	0.00000	0.00000	0.00000	0.00000	0.21415	0.00000
BUTENE-1	1.31358	0.00000	0.00000	0.00000	0.00000	1.31358	0.00000
METHANE	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HYDROGEN	20.25000	0.00000	0.00000	0.00000	0.00000	20.25000	0.00000
NITROGEN	10.25000	0.00000	0.00000	0.00000	0.00000	10.25000	0.00000

OXYGEN BALANCE 99.13501 PERCENT
HYDROGEN BALANCE 97.23388 PERCENT
CARBON BALANCE 64.61411 PERCENT
MATERIAL BALANCE 99.84030 PERCENT

2-BUTANOL COMBUSTION
CONV. TO 1. KETONE 0.00000
2. BUTENES 0.00000

RUN NUMBER 5

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.8	DEG. CENTG.
ATMOPHERIC PRESSURE	701.3	MM HG.
REACTION TEMPERATURE	367.6	DEG. CENTG.
REACTION PRESSURE	703.3	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.03132	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.86493	
INITIAL CONCENTRATION	0.03206	MOLES/LITER

Run number 1

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.8 deg. C.
ATMOSPHERIC PRESSURE	701.3 mm. Hg.
REACTION TEMPERATURE	327.6 deg. C.
REACTION PRESSURE	703.2 mm. Hg.
WT. OF CATALYST	6.8420 gms.
NITROGEN FEED	0.02185 g. per hr.
2-BUTANOL FEED	0.1685 g. per hr.
SPACE VELOCITY	0.0845 hr. ⁻¹
INLET V.	0.4430 l. per hr.
VOLUME CHANGE	0.0443
INITIAL CONCENTRATION	0.0350

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	7.415765	6.384805	12.765075
HYDROGEN	0.175727	0.560635	15.576571
METHANE	0.000000	0.000000	0.000000
BUTENE-1	0.399081	0.376905	0.376288
TRANS-BUTENE-2	0.060019	0.053514	0.053426
CIS-BUTENE-2	0.057580	0.050183	0.050101
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	18.159046	18.032458	14.008818
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	73.248536	74.184938	56.061171
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.484243	0.356558	1.108546
TOTAL	99.999999	99.999999	100.000000

MATERIAL BALANCE	102.559424	PERCENT
CARBON BALANCE	102.277153	PERCENT
HYDROGEN BALANCE	102.914008	PERCENT
OXYGEN BALANCE	103.188633	PERCENT

2-BUTANOL CONVERSION 0.18727
 CONV. TO 1. KETONE 0.20308 2. BUTENES 0.00695

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	12.311309	
HYDROGEN	15.022864	0.205276
METHANE	0.000000	0.000000
BUTENE-1	0.601449	0.008218
TRANS BUTENE-2	0.109946	0.001502
CIS BUTENE-2	0.116209	0.001587
UNKNOWN-1	0.000483	0.000006
METHYL ETHYL KETONE	13.848479	0.189229
1-PROPANOL	0.016309	0.000222
SEC-BUTANOL	56.798994	0.776117
DIETHYL KETONE	0.050817	0.000694
WATER	1.123136	0.015346
TOTAL	100.000000	

MATERIAL BALANCE	97.444311	PERCENT
CARBON BALANCE	97.769031	PERCENT
HYDROGEN BALANCE	98.154492	PERCENT
OXYGEN BALANCE	98.161064	PERCENT

2-BUTANOL CONVERSION 0.22388
 CONV. TO 1. KETONE 0.18922 2. BUTENES 0.01130

COMPOSITIONAL ANALYSIS

COMPOSITIONAL ANALYSIS		PERCENT		WGT. PERCENT	
OXYGEN BALANCE		103.18877		PERCENT	
HYDROGEN BALANCE		102.91402		PERCENT	
CARBON BALANCE		102.27118		PERCENT	
MATERIAL BALANCE		102.25425		PERCENT	
TOTAL		99.99999		WGT. PERCENT	
WATER		0.00000		WGT. PERCENT	
DIETHYL KETONE		0.00000		WGT. PERCENT	
SEC-BUTANOL		33.24838		WGT. PERCENT	
I-PROPANOL		0.00000		WGT. PERCENT	
METHYL ETHYL KETONE		14.12500		WGT. PERCENT	
UNKNOWN-1		0.00000		WGT. PERCENT	
CIS-BUTENE-2		0.00000		WGT. PERCENT	
TRANS-BUTENE-2		0.00000		WGT. PERCENT	
BUTENE-1		0.00000		WGT. PERCENT	
METHANE		0.00000		WGT. PERCENT	
HYDROGEN		0.00000		WGT. PERCENT	
NITROGEN		0.00000		WGT. PERCENT	

CONV. TO 1. KETONE 0.5038 2. BUTENE 0.1857

COMPOSITIONAL ANALYSIS

COMPOSITIONAL ANALYSIS		PERCENT		WGT. PERCENT	
OXYGEN BALANCE		98.11084		PERCENT	
HYDROGEN BALANCE		98.14885		PERCENT	
CARBON BALANCE		97.78031		PERCENT	
MATERIAL BALANCE		97.44231		PERCENT	
TOTAL		100.00000		WGT. PERCENT	
WATER		1.128139		WGT. PERCENT	
DIETHYL KETONE		0.020817		WGT. PERCENT	
SEC-BUTANOL		26.708998		WGT. PERCENT	
I-PROPANOL		0.018309		WGT. PERCENT	
METHYL ETHYL KETONE		13.842476		WGT. PERCENT	
UNKNOWN-1		0.000000		WGT. PERCENT	
CIS-BUTENE-2		0.118309		WGT. PERCENT	
TRANS-BUTENE-2		0.108998		WGT. PERCENT	
BUTENE-1		0.001486		WGT. PERCENT	
METHANE		0.000000		WGT. PERCENT	
HYDROGEN		12.052884		WGT. PERCENT	
NITROGEN		12.371309		WGT. PERCENT	

CONV. TO 1. KETONE 0.1857 2. BUTENE 0.5038

RUN NUMBER 6

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.0	DEG. CENTG.
ATMOPHERIC PRESSURE	701.3	MM HG.
REACTION TEMPERATURE	330.3	DEG. CENTG.
REACTION PRESSURE	703.3	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.02585	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.88299	
INITIAL CONCENTRATION	0.03305	MOLES/LITER

DATE RECEIVED

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	55.0	REF. TEMP.
ATMOSPHERIC PRESSURE	701.3	MM HG.
REACTION TEMPERATURE	330.3	REF. TEMP.
REACTION PRESSURE	703.3	MM HG.
WT. OF CATALYST	0.00200	GRAMS
NITROGEN FEED	0.00280	G. MIN.
2-BUTANOL FEED	0.10050	G. MIN.
SPACE VELOCITY	0.00470	PER HOUR
INSTR.	0.44300	G. MIN.
VOLUME CHANGE	0.88500	
INITIAL CONCENTRATION	0.00300	PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	6.522483	5.608841	13.282633
HYDROGEN	0.010488	0.033421	1.099886
METHANE	0.000000	0.000000	0.000000
BUTENE-1	0.007189	0.006781	0.008019
TRANS-BUTENE-2	0.002760	0.002458	0.002907
CIS-BUTENE-2	0.003062	0.002666	0.003152
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	1.947690	1.931747	1.777592
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	90.967771	92.018020	82.367252
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.538553	0.396062	1.458555
TOTAL	099.999999	100.000000	099.999999

MATERIAL BALANCE	97.162309	PERCENT
CARBON BALANCE	96.779861	PERCENT
HYDROGEN BALANCE	96.956213	PERCENT
OXYGEN BALANCE	98.440958	PERCENT

2-BUTANOL CONVERSION 0.05280
 CONV. TO 1. KETONE 0.02044 2. BUTENES 0.00016

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	13.193584	
HYDROGEN	1.092512	0.012790
METHANE	0.000000	0.000000
BUTENE-1	0.046642	0.000546
TRANS BUTENE-2	0.005185	0.000060
CIS BUTENE-2	0.007998	0.000093
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	1.673151	0.019588
1-PROPANOL	0.011432	0.000133
SEC-BUTANOL	82.451321	0.965325
DIETHYL KETONE	0.058127	0.000680
WATER	1.460044	0.017093
TOTAL	100.000000	

MATERIAL BALANCE	99.142790	PERCENT
CARBON BALANCE	98.656598	PERCENT
HYDROGEN BALANCE	98.832163	PERCENT
OXYGEN BALANCE	100.282280	PERCENT

2-BUTANOL CONVERSION 0.03467
 CONV. TO 1. KETONE 0.01958 2. BUTENES 0.00070

COMPARISON OF THEORETICAL AND ACTUAL

ACTUAL			THEORETICAL		
WATER	0.28822	0.28822	WATER	0.28822	0.28822
DIETHYL KETONE	0.00000	0.00000	DIETHYL KETONE	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	SEC-BUTANOL	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	1-PROPANOL	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	UNKNOWN-1	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	CIS-BUTENE-2	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	TRANS-BUTENE-2	0.00000	0.00000
BUTENE-1	0.00000	0.00000	BUTENE-1	0.00000	0.00000
METHANE	0.00000	0.00000	METHANE	0.00000	0.00000
HYDROGEN	0.00000	0.00000	HYDROGEN	0.00000	0.00000
NITROGEN	0.00000	0.00000	NITROGEN	0.00000	0.00000
TOTAL			TOTAL		
	0.28822	0.28822		0.28822	0.28822
OXYGEN BALANCE	99.4098	PERCENT	OXYGEN BALANCE	99.4098	PERCENT
HYDROGEN BALANCE	98.9851	PERCENT	HYDROGEN BALANCE	98.9851	PERCENT
CARBON BALANCE	97.2791	PERCENT	CARBON BALANCE	97.2791	PERCENT
MATERIAL BALANCE	97.1830	PERCENT	MATERIAL BALANCE	97.1830	PERCENT

CONV. TO 1. KETONE 0.0004 2. BUTENE 0.0015
2-BUTANOL CONVERSION 0.00280

CONVENTIONAL SYSTEM

ACTUAL			THEORETICAL		
WATER	1.2604	0.0815	WATER	1.2604	0.0815
DIETHYL KETONE	0.0000	0.0000	DIETHYL KETONE	0.0000	0.0000
SEC-BUTANOL	82.4131	0.0143	SEC-BUTANOL	82.4131	0.0143
1-PROPANOL	0.0000	0.0000	1-PROPANOL	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	UNKNOWN-1	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	CIS-BUTENE-2	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	TRANS-BUTENE-2	0.0000	0.0000
BUTENE-1	0.0000	0.0000	BUTENE-1	0.0000	0.0000
METHANE	0.0000	0.0000	METHANE	0.0000	0.0000
HYDROGEN	1.0000	0.0000	HYDROGEN	1.0000	0.0000
NITROGEN	13.1358	0.0125	NITROGEN	13.1358	0.0125
TOTAL			TOTAL		
	100.0000			100.0000	
OXYGEN BALANCE	100.2838	PERCENT	OXYGEN BALANCE	100.2838	PERCENT
HYDROGEN BALANCE	98.0313	PERCENT	HYDROGEN BALANCE	98.0313	PERCENT
CARBON BALANCE	98.8888	PERCENT	CARBON BALANCE	98.8888	PERCENT
MATERIAL BALANCE	99.1430	PERCENT	MATERIAL BALANCE	99.1430	PERCENT

CONV. TO 1. KETONE 0.0000 2. BUTENE 0.0000
2-BUTANOL CONVERSION 0.0000

RUN NUMBER 7

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	24.3	DEG. CENTG.
ATMOPHERIC PRESSURE	702.0	MM HG.
REACTION TEMPERATURE	350.9	DEG. CENTG.
REACTION PRESSURE	704.0	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.04374	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.82960	
INITIAL CONCENTRATION	0.03007	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	24.3	°C.
ATMOSPHERIC PRESSURE	765.0	mm. Hg.
REACTION TEMPERATURE	250.0	°C.
REACTION PRESSURE	764.0	mm. Hg.
WT. OF CATALYST	0.0440	GRAM.
NITROGEN FEED	0.0434	G. PER HOUR
2-BUTANOL FEED	0.1632	G. PER HOUR
SPACE VELOCITY	0.0545	PER HOUR
INSTR.	0.4430	G. PER HOUR
VOLUME CHANGE	0.8580	
INITIAL CONCENTRATION	0.0300	MOL PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.449163	9.036581	19.505065
HYDROGEN	0.057475	0.184184	5.524740
METHANE	0.000000	0.000000	0.000000
BUTENE-1	0.024334	0.023085	0.024882
TRANS-BUTENE-2	0.009166	0.008209	0.008848
CIS-BUTENE-2	0.000892	0.000781	0.000841
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	7.669191	7.649666	6.415885
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	81.404439	82.812496	67.563139
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.385336	0.284995	0.956597
TOTAL	99.999999	099.999999	100.000000
MATERIAL BALANCE	98.351644	PERCENT	
CARBON BALANCE	98.087218	PERCENT	
HYDROGEN BALANCE	98.095402	PERCENT	
OXYGEN BALANCE	99.309140	PERCENT	

2-BUTANOL CONVERSION 0.10461
 CONV. TO 1. KETONE 0.08502 2. BUTENES 0.00045

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	17.987432	
HYDROGEN	5.094875	0.065754
METHANE	0.000000	0.000000
BUTENE-1	0.120326	0.001552
TRANS BUTENE-2	0.022112	0.000285
CIS BUTENE-2	0.019475	0.000251
UNKNOWN-1	0.000351	0.000004
METHYL ETHYL KETONE	5.492413	0.070885
1-PROPANOL	0.009274	0.000119
SEC-BUTANOL	70.201431	0.906022
DIETHYL KETONE	0.058354	0.000753
WATER	0.993951	0.012827
TOTAL	100.000000	
MATERIAL BALANCE	97.439006	PERCENT
CARBON BALANCE	98.002857	PERCENT
HYDROGEN BALANCE	98.096781	PERCENT
OXYGEN BALANCE	99.060851	PERCENT

2-BUTANOL CONVERSION 0.09397
 CONV. TO 1. KETONE 0.07088 2. BUTENES 0.00208

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	WGT PERCENT	WGT PERCENT
WATER	0.38385	11.2449	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	81.40449	85.81249	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	7.62101	7.62101	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-2-PENTENE	0.00000	0.00000	0.00000
TRANS-2-PENTENE	0.00000	0.00000	0.00000
2-PENTENE	0.00000	0.00000	0.00000
ETHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	99.99999	99.99999	100.00000
OXYGEN BALANCE	99.99999 PERCENT		
HYDROGEN BALANCE	99.99999 PERCENT		
CARBON BALANCE	99.99999 PERCENT		
MATERIAL BALANCE	99.99999 PERCENT		

CONV. TO 1. KETONE 0.00000 2. BUTENES 0.00000 3. 100.00000

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	WGT PERCENT	WGT PERCENT
WATER	0.00000	0.00000	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	70.20141	70.20141	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	2.43243	2.43243	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-2-PENTENE	0.00000	0.00000	0.00000
TRANS-2-PENTENE	0.00000	0.00000	0.00000
2-PENTENE	0.00000	0.00000	0.00000
ETHANE	0.00000	0.00000	0.00000
HYDROGEN	2.00000	2.00000	0.00000
NITROGEN	17.00000	17.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	99.99999 PERCENT		
HYDROGEN BALANCE	99.99999 PERCENT		
CARBON BALANCE	99.99999 PERCENT		
MATERIAL BALANCE	99.99999 PERCENT		

CONV. TO 1. KETONE 0.00000 2. BUTENES 0.00000 3. 100.00000

RUN NUMBER 8

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.2	DEG. CENTG.
ATMOPHERIC PRESSURE	702.6	MM HG.
REACTION TEMPERATURE	412.7	DEG. CENTG.
REACTION PRESSURE	705.6	MM HG.
WT. OF CATALYST	6.84500	GRAM.
NITROGEN FEED	0.04399	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02472	MOL/HR.G
1/S.V.	40.44303	G.HR./MOL
VOLUME CHANGE	0.82896	
INITIAL CONCENTRATION	0.03027	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.5	deg. C.
ATMOSPHERIC PRESSURE	702.8	mm. Hg.
REACTION TEMPERATURE	412.7	deg. C.
REACTION PRESSURE	705.8	mm. Hg.
WT. OF CATALYST	6.8450	gms.
NITROGEN FEED	0.04349	g. vol. / hr.
S-200ANOL FEED	0.18925	g. vol. / hr.
SPACE VELOCITY	0.05475	ml. / gm. / hr.
1/2 V.	40.44303	g. H ₂ / vol. / hr.
VOLUME CHANGE	0.82804	
INITIAL CONCENTRATION	0.03057	moles / liter

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.549561	9.187931	13.105157
HYDROGEN	0.538666	1.738412	34.458221
METHANE	0.030407	0.018521	0.046137
BUTENE-1	2.649178	2.530897	1.802649
TRANS-BUTENE-2	0.502596	0.453301	0.322867
CIS-BUTENE-2	0.393064	0.346532	0.246820
UNKNOWN-1	0.026020	0.020020	0.017391
METHYL ETHYL KETONE	51.047234	51.277377	28.419809
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	31.848074	32.628089	17.590851
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	2.415195	1.798915	3.990092
TOTAL	099.999999	100.000000	099.999999

MATERIAL BALANCE	97.119279	PERCENT
CARBON BALANCE	95.998174	PERCENT
HYDROGEN BALANCE	99.049345	PERCENT
OXYGEN BALANCE	99.184366	PERCENT

2-BUTANOL CONVERSION 0.65105
 CONV. TO 1. KETONE 0.56375 2. BUTENES 0.04705

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	11.977656	
HYDROGEN	31.493610	0.577796
METHANE	0.042168	0.000773
BUTENE-1	2.140430	0.039269
TRANS BUTENE-2	0.436564	0.008009
CIS BUTENE-2	0.363874	0.006675
UNKNOWN-1	0.052144	0.000956
METHYL ETHYL KETONE	28.876650	0.529784
1-PROPANOL	0.047348	0.000868
SEC-BUTANOL	19.996613	0.366867
DIETHYL KETONE	0.037152	0.000681
WATER	4.535786	0.083215
TOTAL	099.999999	

MATERIAL BALANCE	95.083442	PERCENT
CARBON BALANCE	95.230383	PERCENT
HYDROGEN BALANCE	96.774753	PERCENT
OXYGEN BALANCE	98.141831	PERCENT

2-BUTANOL CONVERSION 0.63313
 CONV. TO 1. KETONE 0.52978 2. BUTENES 0.05395

CONVENTIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
WATER	2.4102	1.70918	2.4102
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	21.88014	38.63804	17.00000
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	21.04388	21.23333	10.00000
UNKNOWN-1	0.02000	0.02000	0.02000
CIS-BUTENE-2	0.38382	0.38382	0.38382
TRANS-BUTENE-2	0.38382	0.38382	0.38382
AVIENE-1	5.84330	5.33000	1.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	99.99999	100.00000	99.99999
OXYGEN BALANCE	99.18325	PERCENT	
HYDROGEN BALANCE	99.04342	PERCENT	
CARBON BALANCE	97.00172	PERCENT	
MATERIAL BALANCE	97.11020	PERCENT	
CONV. TO 1. KETONE 0.0000			
2-BUTANOL CONVERSION	0.0000		

CONVENTIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT
WATER	4.23238	0.00000
DIETHYL KETONE	0.03312	0.00000
SEC-BUTANOL	18.00013	0.00000
1-PROPANOL	0.04380	0.00000
METHYL ETHYL KETONE	28.03660	0.00000
UNKNOWN-1	0.02144	0.00000
CIS-BUTENE-2	0.38382	0.00000
TRANS-BUTENE-2	0.38382	0.00000
AVIENE-1	5.140430	0.00000
METHANE	0.00018	0.00000
HYDROGEN	51.493810	0.00000
NITROGEN	11.07880	0.00000
TOTAL	99.99999	
OXYGEN BALANCE	99.18325	PERCENT
HYDROGEN BALANCE	99.04342	PERCENT
CARBON BALANCE	97.00172	PERCENT
MATERIAL BALANCE	97.00172	PERCENT
CONV. TO 1. KETONE 0.0000		
2-BUTANOL CONVERSION	0.0000	

RUN NUMBER 9

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.8	DEG. CENTG.
ATMOPHERIC PRESSURE	703.0	MM HG.
REACTION TEMPERATURE	345.5	DEG. CENTG.
REACTION PRESSURE	706.0	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.03355	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.85802	
INITIAL CONCENTRATION	0.03178	MOLES/LITER

APPENDIX

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.8	DEG. C. (81.0)
ATMOSPHERIC PRESSURE	703.0	MM. HG.
REACTION TEMPERATURE	345.5	DEG. C. (654.0)
REACTION PRESSURE	708.0	MM. HG.
WT. OF CATALYST	6.9580	GRAMS
NITROGEN FEED	0.0333	G. HOUR
2-BUTANOL FEED	0.1333	G. HOUR
SPACE VELOCITY	0.0333	PER HOUR
HSV	0.1333	PER HOUR
VOLUME CHANGE	0.0280	
INITIAL CONCENTRATION	0.0314	MOL/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	8.350479	7.188787	13.427145
HYDROGEN	0.248081	0.791383	20.541437
METHANE	0.007612	0.004583	0.014950
BUTENE-1	0.095758	0.090428	0.084342
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	21.567936	21.415244	15.542539
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	69.352963	70.231887	49.583038
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.377167	0.277685	0.806546

TOTAL	099.999999	100.000000	100.000000
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MATERIAL BALANCE	96.757573	PERCENT
CARBON BALANCE	96.299555	PERCENT
HYDROGEN BALANCE	97.992511	PERCENT
OXYGEN BALANCE	97.360499	PERCENT

2-BUTANOL CONVERSION 0.26781
 CONV. TO 1. KETONE 0.22951 2. BUTENES 0.00124

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	13.227854	
HYDROGEN	20.236553	0.300447
METHANE	0.014728	0.000218
BUTENE-1	0.130823	0.001942
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.017024	0.000252
METHYL ETHYL KETONE	20.759265	0.308208
1-PROPANOL	0.040669	0.000603
SEC-BUTANOL	44.809340	0.665274
DIETHYL KETONE	0.034844	0.000517
WATER	0.728895	0.010821

TOTAL	099.999999
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MATERIAL BALANCE	97.842875	PERCENT
CARBON BALANCE	97.657984	PERCENT
HYDROGEN BALANCE	97.673727	PERCENT
OXYGEN BALANCE	98.542624	PERCENT

2-BUTANOL CONVERSION 0.33472
 CONV. TO 1. KETONE 0.30820 2. BUTENES 0.00194

COMPOSITIONAL ANALYSIS

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
WATER	0.3717	0.3717	0.3717
DIETHYL KETONE	0.0000	0.0000	0.0000
SEC-BUTANOL	64.3293	70.3717	70.3717
I-PROPANOL	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	31.2727	31.2727	31.2727
UNKNOWN-1	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000
BUTENE-1	0.0000	0.0000	0.0000
METHANE	0.0000	0.0000	0.0000
HYDROGEN	0.2800	0.2800	0.2800
NITROGEN	0.3283	0.3283	0.3283
TOTAL	100.0000	100.0000	100.0000
OXYGEN BALANCE	97.3200		
HYDROGEN BALANCE	97.9211		
CARBON BALANCE	99.2068		
MATERIAL BALANCE	97.2727		
CONV. TO 1. KETONE DIBASE 2. BUTENES DIBASE			
2-BUTANOL CONVERSION			0.2800

COMPOSITIONAL ANALYSIS

COMPONENT	WTF PERCENT	MOLE PERCENT
WATER	0.3717	0.3717
DIETHYL KETONE	0.0000	0.0000
SEC-BUTANOL	64.3293	70.3717
I-PROPANOL	0.0000	0.0000
METHYL ETHYL KETONE	31.2727	31.2727
UNKNOWN-1	0.0170	0.0170
CIS-BUTENE-2	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000
BUTENE-1	0.1308	0.1308
METHANE	0.0142	0.0142
HYDROGEN	0.2800	0.2800
NITROGEN	18.2784	0.3283
TOTAL	100.0000	100.0000
OXYGEN BALANCE	98.2680	
HYDROGEN BALANCE	97.9211	
CARBON BALANCE	97.6796	
MATERIAL BALANCE	97.8485	
CONV. TO 1. KETONE DIBASE 2. BUTENES DIBASE		
2-BUTANOL CONVERSION		0.2800

RUN NUMBER 10

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.7	DEG. CENTG.
ATMOPHERIC PRESSURE	702.6	MM HG.
REACTION TEMPERATURE	367.6	DEG. CENTG.
REACTION PRESSURE	704.6	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04374	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82960	
INITIAL CONCENTRATION	0.03025	MOLES/LITER

THIS REPORT IS

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	DEG. CELSIUS
ATMOSPHERIC PRESSURE	705.0	MM. HG.
REACTION TEMPERATURE	82.5	DEG. CELSIUS
REACTION PRESSURE	704.5	MM. HG.
WT. OF CATALYST	0.0000	GRAMS
NITROGEN FEED	0.0432	G. PER HOUR
S-BUTANOL FEED	0.1032	G. PER HOUR
SPACE VELOCITY	0.0548	PER HOUR
INLET	0.0548	PER HOUR
VOLUME CHANGE	0.0548	
INITIAL CONCENTRATION	0.0502	MOLES PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.302863	8.909517	16.464491
HYDROGEN	0.232138	0.743861	19.103001
METHANE	0.053584	0.032408	0.104590
BUTENE-1	0.422703	0.400970	0.370014
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	24.893054	24.828168	17.828289
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	63.680502	64.778045	45.247301
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.415152	0.307028	0.882309
TOTAL	99.999999	100.000000	100.000000

MATERIAL BALANCE	99.893639	PERCENT
CARBON BALANCE	99.650730	PERCENT
HYDROGEN BALANCE	100.236482	PERCENT
OXYGEN BALANCE	100.413982	PERCENT

2-BUTANOL CONVERSION 0.28961
 CONV. TO 1. KETONE 0.27990 2. BUTENES 0.00580

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	16.296703	
HYDROGEN	18.908324	0.289093
METHANE	0.103525	0.001582
BUTENE-1	0.520666	0.007960
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.015124	0.000231
METHYL ETHYL KETONE	17.247103	0.263694
1-PROPANOL	0.032937	0.000503
SEC-BUTANOL	45.926835	0.702184
DIETHYL KETONE	0.053218	0.000813
WATER	0.895560	0.013692
TOTAL	100.000000	

MATERIAL BALANCE	97.647024	PERCENT
CARBON BALANCE	97.563006	PERCENT
HYDROGEN BALANCE	98.191536	PERCENT
OXYGEN BALANCE	98.088867	PERCENT

2-BUTANOL CONVERSION 0.29781
 CONV. TO 1. KETONE 0.26369 2. BUTENES 0.00796

CONVENTIONAL SYSTEM

COMPONENT		MOLE PERCENT		WGT PERCENT	
TOTAL		99.99999	100.00000	100.00000	
OXYGEN BALANCE		100.01342			PERCENT
HYDROGEN BALANCE		100.23668			PERCENT
CARBON BALANCE		99.85070			PERCENT
MATERIAL BALANCE		99.85239			PERCENT
WATER		0.01115	0.00058	0.00000	
DIETHYL KETONE		0.00000	0.00000	0.00000	
SEC-BUTANOL		63.86005	64.77562	64.77562	
I-PROPANOL		0.00000	0.00000	0.00000	
METHYL ETHYL KETONE		24.86206	25.00000	25.00000	
UNKOWN-1		0.00000	0.00000	0.00000	
CIS-BUTENE-2		0.00000	0.00000	0.00000	
TRANS-BUTENE-2		0.00000	0.00000	0.00000	
BUTENE-1		1.43570	0.00000	0.00000	
METHANE		0.00000	0.00000	0.00000	
HYDROGEN		0.52510	1.00000	1.00000	
NITROGEN		10.00000	8.99999	8.99999	

CONV. TO I. KETONE 0.2390 2. BUTENE-2 0.00000 0.2691

CONVENTIONAL SYSTEM

COMPONENT		MOLE PERCENT		WGT PERCENT	
TOTAL		100.00000			
OXYGEN BALANCE		99.99999			PERCENT
HYDROGEN BALANCE		99.85070			PERCENT
CARBON BALANCE		99.85070			PERCENT
MATERIAL BALANCE		99.85070			PERCENT
WATER		0.00000	0.00000	0.00000	
DIETHYL KETONE		0.00000	0.00000	0.00000	
SEC-BUTANOL		63.86005	64.77562	64.77562	
I-PROPANOL		0.00000	0.00000	0.00000	
METHYL ETHYL KETONE		24.86206	25.00000	25.00000	
UNKOWN-1		0.00000	0.00000	0.00000	
CIS-BUTENE-2		0.00000	0.00000	0.00000	
TRANS-BUTENE-2		0.00000	0.00000	0.00000	
BUTENE-1		1.43570	0.00000	0.00000	
METHANE		0.00000	0.00000	0.00000	
HYDROGEN		0.52510	1.00000	1.00000	
NITROGEN		10.00000	8.99999	8.99999	

CONV. TO I. KETONE 0.2390 2. BUTENE-2 0.00000 0.2691

RUN NUMBER 11

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	DEG. CENTG.
ATMOPHERIC PRESSURE	699.4	MM HG.
REACTION TEMPERATURE	327.3	DEG. CENTG.
REACTION PRESSURE	702.4	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04350	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.83024	
INITIAL CONCENTRATION	0.03017	MOLES/LITER

11. 93800 908

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.0	DEG. CELSIUS
ATMOSPHERIC PRESSURE	699.4	MM. HG.
REACTION TEMPERATURE	327.3	DEG. CELSIUS
REACTION PRESSURE	702.4	MM. HG.
WT. OF CATALYST	0.8280	GRAMS
NITROGEN FEED	0.04350	G. PER MIN.
2-ETHANOL FEED	0.18024	G. PER MIN.
SPACE VELOCITY	0.03980	PER MIN.
12.5 V.	0.21524	G. PER MIN.
VOLUME CHANGE	0.00254	
INITIAL CONCENTRATION	0.00017	MOL PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.472990	9.048795	20.347293
HYDROGEN	0.020507	0.065657	2.051701
METHANE	0.000000	0.000000	0.000000
BUTENE-1	0.013638	0.012925	0.014513
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	2.073430	2.066234	1.805370
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	87.265371	88.692547	75.383053
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.154062	0.113839	0.398066
TOTAL	099.999999	099.999999	100.000000

MATERIAL BALANCE	97.647718	PERCENT
CARBON BALANCE	97.521613	PERCENT
HYDROGEN BALANCE	97.680745	PERCENT
OXYGEN BALANCE	98.006111	PERCENT

2-BUTANOL CONVERSION 0.04777
 CONV. TO 1. KETONE 0.02280 2. BUTENES 0.00018

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	18.520668	
HYDROGEN	1.867515	0.023295
METHANE	0.000000	0.000000
BUTENE-1	0.023856	0.000297
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	2.326340	0.029018
1-PROPANOL	0.037533	0.000468
SEC-BUTANOL	76.745068	0.957305
DIETHYL KETONE	0.073758	0.000920
WATER	0.405258	0.005055
TOTAL	100.000000	

MATERIAL BALANCE	98.103228	PERCENT
CARBON BALANCE	98.812223	PERCENT
HYDROGEN BALANCE	98.772247	PERCENT
OXYGEN BALANCE	99.276680	PERCENT

2-BUTANOL CONVERSION 0.04269
 CONV. TO 1. KETONE 0.02901 2. BUTENES 0.00029

RUN NUMBER 12

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.8	DEG. CENTG.
ATMOPHERIC PRESSURE	698.5	MM HG.
REACTION TEMPERATURE	395.0	DEG. CENTG.
REACTION PRESSURE	701.5	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04847	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.81790	
INITIAL CONCENTRATION	0.02941	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	deg. Cent.
ATMOSPHERIC PRESSURE	698.5	mm. Hg.
REACTION TEMPERATURE	302.5	deg. Cent.
REACTION PRESSURE	701.5	mm. Hg.
WT. OF CATALYST	6.8580	GRAM.
NITROGEN FEED	0.0484	g. MOLYB.
2-BUTANOL FEED	0.1622	g. MOLYB.
SPACE VELOCITY	0.0348	MOLYB./H.
INSTR.	0.8135	g. MOLYB.
VOLUME CHANGE	0.8135	
INITIAL CONCENTRATION	0.0341	MOLYB./LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.623087	10.115461	17.502313
HYDROGEN	0.280896	0.905858	21.781397
METHANE	0.119857	0.072953	0.220446
BUTENE-1	1.117955	1.067255	0.922126
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	41.594133	41.750963	28.070305
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	44.365567	45.418766	29.704060
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.898501	0.668741	1.799350
TOTAL	100.000000	099.999999	099.999999

MATERIAL BALANCE	96.192293	PERCENT
CARBON BALANCE	96.137876	PERCENT
HYDROGEN BALANCE	94.420908	PERCENT
OXYGEN BALANCE	97.483135	PERCENT

2-BUTANOL CONVERSION 0.51393
 CONV. TO 1. KETONE 0.45932 2. BUTENES 0.01508

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	18.290652	
HYDROGEN	22.762474	0.385088
METHANE	0.230375	0.003897
BUTENE-1	1.232005	0.020842
TRANS BUTENE-2	0.001774	0.000030
CIS BUTENE-2	0.004574	0.000077
UNKNOWN-1	0.067155	0.001136
METHYL ETHYL KETONE	26.682213	0.451400
1-PROPANOL	0.087105	0.001473
SEC-BUTANOL	28.828957	0.487718
DIETHYL KETONE	0.066369	0.001122
WATER	1.746340	0.029544
TOTAL	100.000000	

MATERIAL BALANCE	97.566386	PERCENT
CARBON BALANCE	96.355307	PERCENT
HYDROGEN BALANCE	95.238688	PERCENT
OXYGEN BALANCE	97.126037	PERCENT

2-BUTANOL CONVERSION 0.51228
 CONV. TO 1. KETONE 0.45140 2. BUTENES 0.02095

COMPONENT BALANCE SHEET

COMPONENT	UNIT	PERCENT	PERCENT
NITROGEN	1.000000	1.000000	1.000000
HYDROGEN	1.000000	1.000000	1.000000
METHANE	1.000000	1.000000	1.000000
BUTENE-1	1.000000	1.000000	1.000000
TRANS-BUTENE-2	1.000000	1.000000	1.000000
CIS-BUTENE-2	1.000000	1.000000	1.000000
UNKNOWN-1	1.000000	1.000000	1.000000
METHYL ETHYL KETONE	1.000000	1.000000	1.000000
1-PROPANOL	1.000000	1.000000	1.000000
SEC-BUTANOL	1.000000	1.000000	1.000000
DIETHYL KETONE	1.000000	1.000000	1.000000
WATER	1.000000	1.000000	1.000000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	97.45132	PERCENT	
CARBON BALANCE	94.13716	PERCENT	
HYDROGEN BALANCE	94.13716	PERCENT	
NITROGEN BALANCE	94.13716	PERCENT	

CONV. TO 1. KETONE 0.45132 2. BUTENE 0.00000
2-BUTANOL CONVERSION 0.01393

COMPONENT BALANCE SHEET

COMPONENT	UNIT	PERCENT	PERCENT
NITROGEN	1.000000	1.000000	1.000000
HYDROGEN	1.000000	1.000000	1.000000
METHANE	1.000000	1.000000	1.000000
BUTENE-1	1.000000	1.000000	1.000000
TRANS-BUTENE-2	1.000000	1.000000	1.000000
CIS-BUTENE-2	1.000000	1.000000	1.000000
UNKNOWN-1	1.000000	1.000000	1.000000
METHYL ETHYL KETONE	1.000000	1.000000	1.000000
1-PROPANOL	1.000000	1.000000	1.000000
SEC-BUTANOL	1.000000	1.000000	1.000000
DIETHYL KETONE	1.000000	1.000000	1.000000
WATER	1.000000	1.000000	1.000000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	97.13037	PERCENT	
CARBON BALANCE	94.13716	PERCENT	
HYDROGEN BALANCE	94.13716	PERCENT	
NITROGEN BALANCE	94.13716	PERCENT	

CONV. TO 1. KETONE 0.45132 2. BUTENE 0.00000
2-BUTANOL CONVERSION 0.01393

RUN NUMBER 13

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.6	DEG. CENTG.
ATMOPHERIC PRESSURE	698.5	MM HG.
REACTION TEMPERATURE	413.3	DEG. CENTG.
REACTION PRESSURE	702.5	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04549	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82519	
INITIAL CONCENTRATION	0.02984	MOLES/LITER

Run Number 13

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.6	DEG. C
ATMOSPHERIC PRESSURE	698.2	MM HG.
REACTION TEMPERATURE	413.8	DEG. C
REACTION PRESSURE	705.2	MM HG.
WT. OF CATALYST	0.02820	GRAMS
NITROGEN FEED	0.00440	CC. MIN.
2-NUTANIL FEED	0.1632	CC. MIN.
SPACE VELOCITY	11.0348	HR. ⁻¹
INLET V.	40.2152	CC. MIN.
VOLUME CHANGE	0.8521	
INITIAL CONCENTRATION	0.0588	MOLES/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.907142	9.474847	13.241945
HYDROGEN	0.584420	1.881203	36.536841
METHANE	0.315073	0.191421	0.467215
BUTENE-1	1.567704	1.493844	1.042550
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	56.403612	56.511701	30.689430
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	28.352221	28.971663	15.304661
DI-ETHYL KETONE	0.266926	0.284508	0.129322
WATER	1.602898	1.190809	2.588032
TOTAL	99.999999	099.999999	100.000000

MATERIAL BALANCE	97.063180	PERCENT
CARBON BALANCE	96.036145	PERCENT
HYDROGEN BALANCE	99.113863	PERCENT
OXYGEN BALANCE	98.870332	PERCENT

2-BUTANOL CONVERSION 0.68935
 CONV. TO 1. KETONE 0.62290 2. BUTENES 0.02116

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	12.273342	
HYDROGEN	33.864296	0.629406
METHANE	0.433040	0.008048
BUTENE-1	1.276326	0.023721
TRANS BUTENE-2	0.007673	0.000142
CIS BUTENE-2	0.008215	0.000152
UNKNOWN-1	0.190098	0.003533
METHYL ETHYL KETONE	31.914336	0.593164
1-PROPANOL	0.046479	0.000863
SEC-BUTANOL	16.881454	0.313761
DIETHYL KETONE	0.250066	0.004647
WATER	2.854670	0.053057
TOTAL	100.000000	

MATERIAL BALANCE	93.969743	PERCENT
CARBON BALANCE	93.941245	PERCENT
HYDROGEN BALANCE	95.255743	PERCENT
OXYGEN BALANCE	96.549434	PERCENT

2-BUTANOL CONVERSION 0.68623
 CONV. TO 1. KETONE 0.59316 2. BUTENES 0.02401

CONVERSIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
NITROGEN	11.00000	11.00000	11.00000
HYDROGEN	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
BUTENE-1	1.00000	1.00000	1.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
WATER	1.00000	1.00000	1.00000
TOTAL	00.00000	00.00000	00.00000
OXYGEN BALANCE	00.00000	00.00000	00.00000
HYDROGEN BALANCE	00.00000	00.00000	00.00000
CARBON BALANCE	00.00000	00.00000	00.00000
MATERIAL BALANCE	00.00000	00.00000	00.00000

CONV. TO 1. KETONE 0.00000 2. BUTENES 0.00000

CONVERSIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
NITROGEN	12.00000	12.00000	12.00000
HYDROGEN	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
BUTENE-1	1.00000	1.00000	1.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	00.00000	00.00000	00.00000
HYDROGEN BALANCE	00.00000	00.00000	00.00000
CARBON BALANCE	00.00000	00.00000	00.00000
MATERIAL BALANCE	00.00000	00.00000	00.00000

CONV. TO 1. KETONE 0.00000 2. BUTENES 0.00000

RUN NUMBER 14

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.7	DEG. CENTG.
ATMOPHERIC PRESSURE	699.1	MM HG.
REACTION TEMPERATURE	349.9	DEG. CENTG.
REACTION PRESSURE	702.1	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04275	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.83217	
INITIAL CONCENTRATION	0.03024	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	55.1	DEG. CELSIUS
ATMOSPHERIC PRESSURE	760.1	MM HG.
REACTION TEMPERATURE	300.0	DEG. CELSIUS
REACTION PRESSURE	702.1	MM HG.
WT. OF CATALYST	8.8280	GRAM.
NITROGEN FEED	0.0452	G. PER HOUR
2-BUTANOL FEED	0.1652	G. PER HOUR
SPACE VELOCITY	0.0248	PER HOUR
1.2 V.	40.2152	C.H. VOL.
VOLUME CHANGE	0.8317	
INITIAL CONCENTRATION	0.0305	MOL PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.295730	8.899046	18.265307
HYDROGEN	0.116405	0.372828	10.634269
METHANE	0.012578	0.007603	0.027256
BUTENE-1	0.138333	0.131157	0.134428
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	14.740598	14.695071	11.719958
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	74.506314	75.753815	58.770411
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.190038	0.140476	0.448368

TOTAL	099.999999	99.999999	100.000000
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MATERIAL BALANCE	97.749435	PERCENT
CARBON BALANCE	97.686878	PERCENT
HYDROGEN BALANCE	97.479060	PERCENT
OXYGEN BALANCE	98.111649	PERCENT

2-BUTANOL CONVERSION 0.18717
 CONV. TO 1. KETONE 0.16209 2. BUTENES 0.00185

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	17.947507	
HYDROGEN	10.449242	0.144179
METHANE	0.026782	0.000369
BUTENE-1	0.161559	0.002229
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	8.837815	0.121945
1-PROPANOL	0.039781	0.000548
SEC-BUTANOL	62.063817	0.856363
DIETHYL KETONE	0.000000	0.000000
WATER	0.473494	0.006533

TOTAL	100.000000
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MATERIAL BALANCE	98.245096	PERCENT
CARBON BALANCE	98.104189	PERCENT
HYDROGEN BALANCE	98.643253	PERCENT
OXYGEN BALANCE	98.539085	PERCENT

2-BUTANOL CONVERSION 0.14363
 CONV. TO 1. KETONE 0.12194 2. BUTENES 0.00222

CONVENTIONAL SYSTEM

COMPONENT			MATERIAL BALANCE		
NITROGEN			PERCENT		
HYDROGEN			PERCENT		
METHANE			PERCENT		
BUTENE-1			PERCENT		
TRANS BUTENE-2			PERCENT		
CIS BUTENE-2			PERCENT		
UNKNOWN-1			PERCENT		
METHYL ETHYL KETONE			PERCENT		
I-PROPANOL			PERCENT		
SEC-BUTANOL			PERCENT		
DIETHYL KETONE			PERCENT		
WATER			PERCENT		
TOTAL			PERCENT		

CONV. TO I. KETONE 0.1825 2. BUTENES 0.0145
2-BUTANOL CONVERSION 0.1825

CONVENTIONAL SYSTEM

COMPONENT			MATERIAL BALANCE		
NITROGEN			PERCENT		
HYDROGEN			PERCENT		
METHANE			PERCENT		
BUTENE-1			PERCENT		
TRANS BUTENE-2			PERCENT		
CIS BUTENE-2			PERCENT		
UNKNOWN-1			PERCENT		
METHYL ETHYL KETONE			PERCENT		
I-PROPANOL			PERCENT		
SEC-BUTANOL			PERCENT		
DIETHYL KETONE			PERCENT		
WATER			PERCENT		
TOTAL			PERCENT		

CONV. TO I. KETONE 0.1825 2. BUTENES 0.0145
2-BUTANOL CONVERSION 0.1825

RUN NUMBER 15

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	DEG. CENTG.
ATMOPHERIC PRESSURE	699.2	MM HG.
REACTION TEMPERATURE	386.4	DEG. CENTG.
REACTION PRESSURE	702.2	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04126	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.83610	
INITIAL CONCENTRATION	0.03048	MOLES/LITER

ROOM NUMBER 10

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	DEG. CELSIUS
ATMOSPHERIC PRESSURE	699.5	MM HG.
REACTION TEMPERATURE	386.4	DEG. CELSIUS
REACTION PRESSURE	705.5	MM HG.
WT. OF CATALYST	2.8200	GRAM.
NITROGEN FEED	0.04150	G. BOLLER
2-NUTAMOL FEED	0.10550	G. BOLLER
SPACE VELOCITY	0.05480	BOLLER
1/2. V.	40.5150	G. HH. VAPOR
VOLUME CHANGE	0.8310	
INITIAL CONCENTRATION	0.03040	BOLLER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	9.783204	8.464247	14.622795
HYDROGEN	0.317925	1.019252	24.470319
METHANE	0.136875	0.082822	0.249884
BUTENE-1	0.674975	0.640582	0.552623
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	36.530947	36.453429	24.470977
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	52.022631	52.944963	34.573028
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.533440	0.394700	1.060371
TOTAL	99.999999	100.000000	099.999999

MATERIAL BALANCE	99.659078	PERCENT
CARBON BALANCE	99.469524	PERCENT
HYDROGEN BALANCE	99.701113	PERCENT
OXYGEN BALANCE	100.211934	PERCENT

2-BUTANOL CONVERSION 0.42356
 CONV. TO 1. KETONE 0.40800 2. BUTENES 0.00921

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	14.385023	
HYDROGEN	24.072423	0.385431
METHANE	0.245821	0.003935
BUTENE-1	0.739902	0.011846
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	23.808252	0.381201
1-PROPANOL	0.061538	0.000985
SEC-BUTANOL	35.595312	0.569927
DIETHYL KETONE	0.000000	0.000000
WATER	1.091725	0.017479
TOTAL	100.000000	

MATERIAL BALANCE	96.424143	PERCENT
CARBON BALANCE	96.469909	PERCENT
HYDROGEN BALANCE	96.731132	PERCENT
OXYGEN BALANCE	96.959458	PERCENT

2-BUTANOL CONVERSION 0.43007
 CONV. TO 1. KETONE 0.38120 2. BUTENES 0.01184

CONVENTIONAL SYSTEM

COMPONENT		WGT. PERCENT		VOL. PERCENT	
WATER		0.83440	0.83440	0.83440	0.83440
DIETHYL KETONE		0.00000	0.00000	0.00000	0.00000
SEC-BUTANOL		22.02231	22.02231	22.02231	22.02231
I-PROPANOL		0.00000	0.00000	0.00000	0.00000
METHYL ETHYL KETONE		34.55045	34.55045	34.55045	34.55045
UNKNOWN-1		0.00000	0.00000	0.00000	0.00000
CIS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
TRANS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
BUTENE-1		0.64274	0.64274	0.64274	0.64274
METHANE		0.13485	0.13485	0.13485	0.13485
HYDROGEN		0.21271	0.21271	0.21271	0.21271
NITROGEN		0.17450	0.17450	0.17450	0.17450
TOTAL		99.86660	100.00000	100.00000	100.00000
OXYGEN BALANCE		100.2134	PERCENT		
HYDROGEN BALANCE		99.70113	PERCENT		
CARBON BALANCE		99.46024	PERCENT		
MATERIAL BALANCE		99.46024	PERCENT		
CONV. TO I. KETONE 0.0000					
2-BUTANOL CONVERSION		0.43356			

CONVENTIONAL SYSTEM

COMPONENT		WGT. PERCENT		VOL. PERCENT	
WATER		1.00125	0.81250	0.81250	0.81250
DIETHYL KETONE		0.00000	0.00000	0.00000	0.00000
SEC-BUTANOL		32.82215	32.82215	32.82215	32.82215
I-PROPANOL		0.00125	0.00125	0.00125	0.00125
METHYL ETHYL KETONE		23.80225	23.80225	23.80225	23.80225
UNKNOWN-1		0.00000	0.00000	0.00000	0.00000
CIS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
TRANS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
BUTENE-1		0.73605	0.73605	0.73605	0.73605
METHANE		0.24821	0.24821	0.24821	0.24821
HYDROGEN		54.07243	54.07243	54.07243	54.07243
NITROGEN		14.38253	14.38253	14.38253	14.38253
TOTAL		100.00000	100.00000	100.00000	100.00000
OXYGEN BALANCE		99.82442	PERCENT		
HYDROGEN BALANCE		99.71132	PERCENT		
CARBON BALANCE		99.46024	PERCENT		
MATERIAL BALANCE		99.46024	PERCENT		
CONV. TO I. KETONE 0.8125					
2-BUTANOL CONVERSION		0.43007			

RUN NUMBER 16

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	694.4	MM HG.
REACTION TEMPERATURE	366.7	DEG. CENTG.
REACTION PRESSURE	696.4	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04549	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82519	
INITIAL CONCENTRATION	0.02963	MOLES/LITER

Run Number 16

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CELC.
ATMOSPHERIC PRESSURE	696.4	MM HG.
REACTION TEMPERATURE	266.7	DEG. CELC.
REACTION PRESSURE	696.4	MM HG.
WT. OF CATALYST	6.8560	GRAM.
NITROGEN FEED	0.0448	G. PER HR.
S-BUTANOL FEED	0.1638	G. PER HR.
SPACE VELOCITY	0.0246	PER HOUR
I.V.	40.8125	G. PER LITER
VOLUME CHANGE	0.8219	
INITIAL CONCENTRATION	0.0363	MOLE/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.979198	9.495546	17.400393
HYDROGEN	0.238882	0.765565	19.495629
METHANE	0.057819	0.034973	0.111925
BUTENE-1	0.374922	0.355689	0.325478
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.006339	0.004843	0.005406
METHYL ETHYL KETONE	24.134579	24.074612	17.142308
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	64.013408	65.124648	45.108172
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.194849	0.144119	0.410686
TOTAL	99.999999	99.999999	100.000000
MATERIAL BALANCE	96.829448	PERCENT	
CARBON BALANCE	96.700637	PERCENT	
HYDROGEN BALANCE	97.479900	PERCENT	
OXYGEN BALANCE	96.789032	PERCENT	

2-BUTANOL CONVERSION 0.30324
 CONV. TO 1. KETONE 0.26478 2. BUTENES 0.00502

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	16.629871	
HYDROGEN	18.632326	0.283196
METHANE	0.106968	0.001625
BUTENE-1	0.430999	0.006550
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	16.761418	0.254759
1-PROPANOL	0.054928	0.000834
SEC-BUTANOL	46.955976	0.713692
DIETHYL KETONE	0.000000	0.000000
WATER	0.427509	0.006497
TOTAL	100.000000	
MATERIAL BALANCE	97.337729	PERCENT
CARBON BALANCE	97.603612	PERCENT
HYDROGEN BALANCE	98.199839	PERCENT
OXYGEN BALANCE	97.578534	PERCENT

2-BUTANOL CONVERSION 0.28630
 CONV. TO 1. KETONE 0.25475 2. BUTENES 0.00655

COMPOSITIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
NITROGEN	10.17418	0.43250	0.43250
HYDROGEN	0.23432	0.00000	0.00000
METHANE	0.02482	0.00000	0.00000
BUTENE-1	0.37432	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00330	0.00408	0.00408
METHYL ETHYL KETONE	24.13428	0.00000	0.00000
I-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.01348	0.00000	0.00000
DI-ETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.10448	0.00000	0.00000
TOTAL	99.99999	99.99999	99.99999
OXYGEN BALANCE	99.99999	PERCENT	PERCENT
CARBON BALANCE	99.99999	PERCENT	PERCENT
HYDROGEN BALANCE	99.99999	PERCENT	PERCENT
MATERIAL BALANCE	99.99999	PERCENT	PERCENT

CONV. TO I. KETONE 0.5418 2. BUTENES 0.00000
2-BUTANOL CONVERSION 0.50324

COMPOSITIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
NITROGEN	10.17418	0.43250	0.43250
HYDROGEN	0.23432	0.00000	0.00000
METHANE	0.02482	0.00000	0.00000
BUTENE-1	0.37432	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00330	0.00408	0.00408
METHYL ETHYL KETONE	24.13428	0.00000	0.00000
I-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.01348	0.00000	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.10448	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	99.99999	PERCENT	PERCENT
CARBON BALANCE	99.99999	PERCENT	PERCENT
HYDROGEN BALANCE	99.99999	PERCENT	PERCENT
MATERIAL BALANCE	99.99999	PERCENT	PERCENT

CONV. TO I. KETONE 0.5418 2. BUTENES 0.00000
2-BUTANOL CONVERSION 0.50324

RUN NUMBER 17

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.8	DEG. CENTG.
ATMOPHERIC PRESSURE	698.6	MM HG.
REACTION TEMPERATURE	331.5	DEG. CENTG.
REACTION PRESSURE	700.6	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04698	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82150	
INITIAL CONCENTRATION	0.02952	MOLES/LITER

Run number 15

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.8	DEG. CELSIUS
ATMOSPHERIC PRESSURE	698.6	MM HG.
REACTION TEMPERATURE	131.8	DEG. CELSIUS
REACTION PRESSURE	700.0	MM HG.
WT. OF CATALYST	2.8300	GRAMS
NITROGEN FEED	0.0488	G. MOLE/HR.
2-BUTANOL FEED	0.1852	G. MOLE/HR.
SPACE VELOCITY	0.0548	MOLE/HR. G.
INSTR.	40.815	G. HR. VOLUME
VOLUME CHANGE	0.8312	
INITIAL CONCENTRATION	0.0525	MOLE/HR. G.

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.438784	9.900645	22.023009
HYDROGEN	0.019294	0.061881	1.912895
METHANE	0.000000	0.000000	0.000000
BUTENE-1	0.012425	0.011797	0.013104
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	3.550154	3.544060	3.063269
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	84.837212	86.376408	72.623806
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.142128	0.105205	0.363914
TOTAL	100.000000	100.000000	100.000000

MATERIAL BALANCE	95.483060	PERCENT
CARBON BALANCE	95.415229	PERCENT
HYDROGEN BALANCE	95.213669	PERCENT
OXYGEN BALANCE	95.857403	PERCENT

2-BUTANOL CONVERSION 0.08462
 CONV. TO 1. KETONE 0.03861 2. BUTENES 0.00016

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	22.249839	
HYDROGEN	1.932598	0.025267
METHANE	0.000000	0.000000
BUTENE-1	0.016812	0.000219
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	2.053534	0.026849
1-PROPANOL	0.011901	0.000155
SEC-BUTANOL	73.367671	0.959253
DIETHYL KETONE	0.000000	0.000000
WATER	0.367642	0.004806
TOTAL	100.000000	

MATERIAL BALANCE	99.320994	PERCENT
CARBON BALANCE	98.643885	PERCENT
HYDROGEN BALANCE	98.704778	PERCENT
OXYGEN BALANCE	99.106471	PERCENT

2-BUTANOL CONVERSION 0.04074
 CONV. TO 1. KETONE 0.02684 2. BUTENES 0.00021

COMBUSTION CALCULATIONS

COMPONENT	MOLE PERCENT	WEIGHT PERCENT	MOLE PERCENT
NITROGEN	11.8371	0.0000	0.0000
HYDROGEN	0.0100	0.0000	0.0000
METHANE	0.0000	0.0000	0.0000
BUTENE-1	0.0155	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	3.5012	0.0000	0.0000
I-PROPANOL	0.0000	0.0000	0.0000
SEC-BUTANOL	0.0000	0.0000	0.0000
DI-ETHYL KETONE	0.0000	0.0000	0.0000
WATER	0.1412	0.0000	0.0000
TOTAL	100.0000	100.0000	100.0000

OXYGEN BALANCE	92.82403 PERCENT
HYDROGEN BALANCE	92.51346 PERCENT
CARBON BALANCE	92.41239 PERCENT
MATERIAL BALANCE	92.48300 PERCENT

CONV. TO I. KETONE 0.0000 2. BUTENE 0.0000
S-BUTANOL CONVERSION 0.0846

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	WEIGHT PERCENT
NITROGEN	22.94039	0.0000
HYDROGEN	1.93298	0.0000
METHANE	0.00000	0.0000
BUTENE-1	0.01612	0.0000
TRANS BUTENE-2	0.00000	0.0000
CIS BUTENE-2	0.00000	0.0000
UNKNOWN-1	0.00000	0.0000
METHYL ETHYL KETONE	2.02334	0.0000
I-PROPANOL	0.01101	0.0000
SEC-BUTANOL	13.36151	0.0000
DIETHYL KETONE	0.00000	0.0000
WATER	0.36185	0.0000
TOTAL	100.00000	100.0000

OXYGEN BALANCE	99.10471 PERCENT
HYDROGEN BALANCE	98.70478 PERCENT
CARBON BALANCE	99.64385 PERCENT
MATERIAL BALANCE	99.32054 PERCENT

CONV. TO I. KETONE 0.0000 2. BUTENE 0.0000
S-BUTANOL CONVERSION 0.0846

RUN NUMBER 18

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	24.5	DEG. CENTG.
ATMOPHERIC PRESSURE	701.3	MM HG.
REACTION TEMPERATURE	346.0	DEG. CENTG.
REACTION PRESSURE	704.3	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04549	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82519	
INITIAL CONCENTRATION	0.02977	MOLES/LITER

RUN NUMBER 18

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	24.5	DEG. CELSIUS
ATMOSPHERIC PRESSURE	701.3	MM HG.
REACTION TEMPERATURE	346.0	DEG. CELSIUS
REACTION PRESSURE	704.3	MM HG.
WT. OF CATALYST	8.8680	GRAM.
NITROGEN FEED	0.04248	L. PER HOUR
2-BUTANOL FEED	0.16252	L. PER HOUR
SPACE VELOCITY	0.02468	PER HOUR
INLET	0.51215	PER HOUR
VOLUME CHANGE	0.82519	
INITIAL CONCENTRATION	0.02477	PER HOUR

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.713447	9.265739	19.417450
HYDROGEN	0.089214	0.285915	8.326562
METHANE	0.008040	0.004863	0.017799
BUTENE-1	0.112401	0.106635	0.111590
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	12.132807	12.102703	9.855197
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	76.778709	78.111820	61.872774
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.165378	0.122322	0.398625
TOTAL	099.999999	100.000000	100.000000

MATERIAL BALANCE	99.482954	PERCENT
CARBON BALANCE	99.445496	PERCENT
HYDROGEN BALANCE	99.105470	PERCENT
OXYGEN BALANCE	99.836646	PERCENT

2-BUTANOL CONVERSION 0.14356
 CONV. TO 1. KETONE 0.13641 2. BUTENES 0.00154

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	18.973078	
HYDROGEN	8.136007	0.109787
METHANE	0.017392	0.000234
BUTENE-1	0.163368	0.002204
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.008331	0.000112
METHYL ETHYL KETONE	7.895514	0.106542
1-PROPANOL	0.045808	0.000618
SEC-BUTANOL	64.345938	0.868284
DIETHYL KETONE	0.000000	0.000000
WATER	0.414559	0.005594
TOTAL	100.000000	

MATERIAL BALANCE	97.611243	PERCENT
CARBON BALANCE	97.755331	PERCENT
HYDROGEN BALANCE	97.894637	PERCENT
OXYGEN BALANCE	98.103873	PERCENT

2-BUTANOL CONVERSION 0.13171
 CONV. TO 1. KETONE 0.10654 2. BUTENES 0.00220

CONVENTIONAL SYSTEM

COMPONENT	WEIGHT PERCENT	MOLE PERCENT	WT. FRACTION
WATER	0.15238	0.15238	0.15238
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	26.23209	26.23209	26.23209
I-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	12.13209	12.13209	12.13209
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.11209	0.11209	0.11209
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	99.83668	PERCENT	
HYDROGEN BALANCE	99.10240	PERCENT	
CARBON BALANCE	99.46298	PERCENT	
MATERIAL BALANCE	99.46298	PERCENT	
CONV. TO 1. KETONE 0.13841	2. BUTENES 0.0015		
2-BUTANOL CONVERSION	0.13841		

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	WT. FRACTION
WATER	0.15238	0.15238
DIETHYL KETONE	0.00000	0.00000
SEC-BUTANOL	26.23209	26.23209
I-PROPANOL	0.00000	0.00000
METHYL ETHYL KETONE	12.13209	12.13209
UNKNOWN-1	0.00000	0.00000
CIS BUTENE-2	0.00000	0.00000
TRANS BUTENE-2	0.00000	0.00000
BUTENE-1	0.11209	0.11209
METHANE	0.00000	0.00000
HYDROGEN	0.00000	0.00000
NITROGEN	0.00000	0.00000
TOTAL	100.00000	100.00000
OXYGEN BALANCE	99.10240	PERCENT
HYDROGEN BALANCE	97.29667	PERCENT
CARBON BALANCE	97.35231	PERCENT
MATERIAL BALANCE	97.61243	PERCENT
CONV. TO 1. KETONE 0.1055	2. BUTENES 0.0015	
2-BUTANOL CONVERSION	0.13111	

RUN NUMBER 19

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	30.0	DEG. CENTG.
ATMOPHERIC PRESSURE	701.2	MM HG.
REACTION TEMPERATURE	367.0	DEG. CENTG.
REACTION PRESSURE	705.2	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04847	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.81790	
INITIAL CONCENTRATION	0.02883	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	30.0 DEG. CENT.
ATMOSPHERIC PRESSURE	761.5 MM. HG.
REACTION TEMPERATURE	347.0 DEG. CENT.
REACTION PRESSURE	702.5 MM. HG.
WT. OF CATALYST	4.3580 GRAM.
NITROGEN FEED	0.04847 G. MIN.
S-BUTANOL FEED	0.1625 G. MIN.
SPACE VELOCITY	0.02468 MIN. ⁻¹
INLET	40.5152 G. MIN.
VOLUME CHANGE	0.8138
INITIAL CONCENTRATION	0.02898 MOL/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.587418	10.037735	18.443481
HYDROGEN	0.224938	0.722041	18.436780
METHANE	0.054248	0.032866	0.105464
BUTENE-1	0.381859	0.362854	0.332929
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	24.514557	24.493077	17.487244
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	62.924012	64.119566	44.531616
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.312965	0.231857	0.662483
TOTAL	100.000000	099.999999	100.000000

MATERIAL BALANCE	97.020973	PERCENT
CARBON BALANCE	96.863443	PERCENT
HYDROGEN BALANCE	97.285254	PERCENT
OXYGEN BALANCE	97.334247	PERCENT

2-BUTANOL CONVERSION 0.30849
 CONV. TO 1. KETONE 0.27154 2. BUTENES 0.00516

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	18.051978	
HYDROGEN	18.045419	0.276587
METHANE	0.103225	0.001582
BUTENE-1	0.444461	0.006812
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.016673	0.000255
METHYL ETHYL KETONE	16.947929	0.259765
1-PROPANOL	0.055060	0.000843
SEC-BUTANOL	45.654932	0.699766
DIETHYL KETONE	0.001124	0.000017
WATER	0.679195	0.010410
TOTAL	100.000000	

MATERIAL BALANCE	96.854587	PERCENT
CARBON BALANCE	96.739485	PERCENT
HYDROGEN BALANCE	97.175394	PERCENT
OXYGEN BALANCE	97.080382	PERCENT

2-BUTANOL CONVERSION 0.30023
 CONV. TO 1. KETONE 0.25976 2. BUTENES 0.00681

CONVENTIONAL SYSTEM

COMPONENT		WGT. PERCENT		WGT. PERCENT	
WATER		0.21205	0.21205	0.21205	0.21205
DIETHYL KETONE		0.00000	0.00000	0.00000	0.00000
SEC-BUTANOL		0.23403	0.23403	0.23403	0.23403
1-PROPANOL		0.00000	0.00000	0.00000	0.00000
METHYL ETHYL KETONE		0.00000	0.00000	0.00000	0.00000
UNKNOWN-1		0.00000	0.00000	0.00000	0.00000
CIS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
TRANS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
BUTENE-1		0.20198	0.20198	0.20198	0.20198
ETHANE		0.02328	0.02328	0.02328	0.02328
HYDROGEN		0.23403	0.23403	0.23403	0.23403
NITROGEN		11.28141	11.28141	11.28141	11.28141
TOTAL		100.00000	100.00000	100.00000	100.00000
OXYGEN BALANCE		0.33424	PERCENT		
HYDROGEN BALANCE		0.28224	PERCENT		
CARBON BALANCE		0.43443	PERCENT		
MATERIAL BALANCE		0.02003	PERCENT		

CONV. TO 1. KETONE 0.21205 2. BUTENES 0.00000
2-BUTANOL CONVERSION 0.40848

CONVENTIONAL SYSTEM

COMPONENT		WGT. PERCENT		WGT. PERCENT	
WATER		0.21205	0.21205	0.21205	0.21205
DIETHYL KETONE		0.00114	0.00114	0.00114	0.00114
SEC-BUTANOL		0.23403	0.23403	0.23403	0.23403
1-PROPANOL		0.00000	0.00000	0.00000	0.00000
METHYL ETHYL KETONE		1.24415	1.24415	1.24415	1.24415
UNKNOWN-1		0.01673	0.01673	0.01673	0.01673
CIS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
TRANS-BUTENE-2		0.00000	0.00000	0.00000	0.00000
BUTENE-1		0.44461	0.44461	0.44461	0.44461
ETHANE		0.10322	0.10322	0.10322	0.10322
HYDROGEN		1.24415	1.24415	1.24415	1.24415
NITROGEN		18.02198	18.02198	18.02198	18.02198
TOTAL		100.00000	100.00000	100.00000	100.00000
OXYGEN BALANCE		0.00382	PERCENT		
HYDROGEN BALANCE		0.12588	PERCENT		
CARBON BALANCE		0.23042	PERCENT		
MATERIAL BALANCE		0.00294	PERCENT		

CONV. TO 1. KETONE 0.20840 2. BUTENES 0.00000
2-BUTANOL CONVERSION 0.80053

RUN NUMBER 20

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	699.5	MM HG.
REACTION TEMPERATURE	394.6	DEG. CENTG.
REACTION PRESSURE	702.5	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04698	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82150	
INITIAL CONCENTRATION	0.02964	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	55.0	DEG. CELSIUS
ATMOSPHERIC PRESSURE	699.5	MM. HG.
REACTION TEMPERATURE	304.6	DEG. CELSIUS
REACTION PRESSURE	702.5	MM. HG.
MT. OF CATALYST	6.8580	GRAMS
NITROGEN FEED	0.0000	L. PER MIN.
2-BUTANOL FEED	0.1035	L. PER MIN.
SPACE VELOCITY	0.0249	PER MIN.
INLET V.	60.5135	L. PER MIN.
VOLUME CHANGE	0.8510	
INITIAL CONCENTRATION	0.0284	WEIGHT PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.378646	9.870698	15.730106
HYDROGEN	0.401474	1.290518	28.580098
METHANE	0.182863	0.110943	0.308768
BUTENE-1	0.977777	0.930415	0.740411
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	41.693261	41.715110	25.831406
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	44.610623	45.521932	27.420489
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.755353	0.560380	1.388719
TOTAL	99.999999	099.999999	099.999999

MATERIAL BALANCE	95.804586	PERCENT
CARBON BALANCE	95.415325	PERCENT
HYDROGEN BALANCE	96.695979	PERCENT
OXYGEN BALANCE	96.423161	PERCENT

2-BUTANOL CONVERSION 0.51611
 CONV. TO 1. KETONE 0.45584 2. BUTENES 0.01306

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	14.875994	
HYDROGEN	27.028257	0.459479
METHANE	0.292002	0.004964
BUTENE-1	0.929029	0.015793
TRANS BUTENE-2	0.004320	0.000073
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	26.344110	0.447848
1-PROPANOL	0.071074	0.001208
SEC-BUTANOL	28.963698	0.492381
DIETHYL KETONE	0.024635	0.000418
WATER	1.466875	0.024936
TOTAL	100.000000	

MATERIAL BALANCE	95.632863	PERCENT
CARBON BALANCE	95.876837	PERCENT
HYDROGEN BALANCE	96.360877	PERCENT
OXYGEN BALANCE	96.679464	PERCENT

2-BUTANOL CONVERSION 0.50761
 CONV. TO 1. KETONE 0.44784 2. BUTENES 0.01586

CONVENTIONAL SYSTEM

COMPONENT	WGT. PERCENT	WGT. PERCENT	WGT. PERCENT
WATER	0.75523	0.75523	1.77277
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	44.41023	44.41023	27.42082
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	41.61341	41.61341	25.77119
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.97777	0.97777	0.97777
ETHANE	0.13263	0.13263	0.13263
HYDROGEN	0.41474	1.00000	29.60000
NITROGEN	11.37044	11.37044	11.37044
TOTAL	99.99999	99.99999	100.00000
OXYGEN BALANCE	98.423161	PERCENT	
HYDROGEN BALANCE	96.69279	PERCENT	
CARBON BALANCE	95.41525	PERCENT	
MATERIAL BALANCE	95.80254	PERCENT	
CONV. TO 1. KETONE 0.45284	2. BUTENE2 0.01208		
2-BUTANOL CONVERSION	0.51611		

CONVENTIONAL SYSTEM

COMPONENT	WGT. PERCENT	WGT. PERCENT	WGT. PERCENT
WATER	1.466825	0.024635	0.000000
DIETHYL KETONE	0.024635	0.024635	0.000000
SEC-BUTANOL	20.963698	0.071074	0.001200
1-PROPANOL	0.071074	0.071074	0.001200
METHYL ETHYL KETONE	26.344110	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000	0.000000
TRANS BUTENE-2	0.004320	0.000000	0.000000
BUTENE-1	0.920029	0.012798	0.000000
METHANE	0.292002	0.000000	0.000000
HYDROGEN	27.028227	20.629410	0.000000
NITROGEN	14.872304		
TOTAL	100.00000		
OXYGEN BALANCE	96.51044	PERCENT	
HYDROGEN BALANCE	96.20827	PERCENT	
CARBON BALANCE	95.47887	PERCENT	
MATERIAL BALANCE	95.43263	PERCENT	
CONV. TO 1. KETONE 0.45284	2. BUTENE2 0.01208		
2-BUTANOL CONVERSION	0.50701		

RUN NUMBER 21

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	DEG. CENTG.
ATMOPHERIC PRESSURE	698.7	MM HG.
REACTION TEMPERATURE	414.0	DEG. CENTG.
REACTION PRESSURE	702.7	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04847	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.81790	
INITIAL CONCENTRATION	0.02945	MOLES/LITER

WATER NUMBER 14

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.5 DEG. CELSIUS
ATMOSPHERIC PRESSURE	698.7 MM. HG.
REACTION TEMPERATURE	414.0 DEG. CELSIUS
REACTION PRESSURE	702.7 MM. HG.
WT. OF CATALYST	6.6288 GRAM.
NITROGEN FEED	0.06847 G. MINUTE
2-BUTANOL FEED	0.1652 G. MINUTE
SPACE VELOCITY	0.0266 LITERS/GRAM-HR.
1/2 V.	0.21575 G. HR. VOLUME
WATER CHANGE	0.21700
INITIAL CONCENTRATION	0.02445 MOLES/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.665415	10.144447	14.377119
HYDROGEN	0.556715	1.793952	35.332152
METHANE	0.320524	0.194942	0.482500
BUTENE-1	1.497746	1.428717	1.011118
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.039557	0.030390	0.026231
METHYL ETHYL KETONE	56.186744	56.354980	31.034636
1-PROPANOL	0.036829	0.036154	0.023885
SEC-BUTANOL	28.135950	28.781597	15.418038
DI-ETHYL KETONE	0.229649	0.245039	0.112948
WATER	1.330865	0.989777	2.181367
TOTAL	099.999999	100.000000	100.000000

MATERIAL BALANCE	95.886510	PERCENT
CARBON BALANCE	95.107069	PERCENT
HYDROGEN BALANCE	97.375775	PERCENT
OXYGEN BALANCE	97.153609	PERCENT

2-BUTANOL CONVERSION 0.69286
 CONV. TO 1. KETONE 0.61822 2. BUTENES 0.02014

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	13.607668	
HYDROGEN	33.441206	0.625403
METHANE	0.456677	0.008540
BUTENE-1	1.215644	0.022734
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.019256	0.000360
METHYL ETHYL KETONE	31.630131	0.591533
1-PROPANOL	0.006608	0.000123
SEC-BUTANOL	17.047744	0.318819
DIETHYL KETONE	0.163121	0.003050
WATER	2.411941	0.045107
TOTAL	099.999999	

MATERIAL BALANCE	93.955708	PERCENT
CARBON BALANCE	93.912826	PERCENT
HYDROGEN BALANCE	95.090138	PERCENT
OXYGEN BALANCE	95.863398	PERCENT

2-BUTANOL CONVERSION 0.68118
 CONV. TO 1. KETONE 0.59153 2. BUTENES 0.02273

COMBUSTION ANALYSIS

Component	Weight Percent	Volume Percent	Weight Percent
WATER	1.33085	0.00477	2.11307
DIETHYL KETONE	0.32849	0.00179	0.11529
SEC-BUTANOL	0.13220	0.00197	0.00000
1-PROPANOL	0.03829	0.00000	0.00000
METHYL ETHYL KETONE	0.11744	0.00000	0.00000
UNKNOWN-1	0.03227	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	1.48708	1.00000	0.00000
METHANE	0.12023	0.00000	0.00000
NITROGEN	0.22972	1.00000	0.00000
HYDROGEN	1.00000	1.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	97.12309	PERCENT	
HYDROGEN BALANCE	97.37272	PERCENT	
CARBON BALANCE	92.10709	PERCENT	
MATERIAL BALANCE	92.88210	PERCENT	

CONV. TO 1. KETONE 0.4122 2. BUTENE 0.0511
5-BUTANOL CONVERSION 0.00589

COMBUSTION ANALYSIS

Component	Weight Percent	Volume Percent	Weight Percent
WATER	2.41241	0.00197	0.00000
DIETHYL KETONE	0.13211	0.00000	0.00000
SEC-BUTANOL	1.00734	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	1.18013	0.00000	0.00000
UNKNOWN-1	0.01220	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	1.22844	0.00000	0.00000
METHANE	0.42477	0.00000	0.00000
HYDROGEN	33.41220	0.00000	0.00000
NITROGEN	18.60768	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	92.00320	PERCENT	
HYDROGEN BALANCE	92.00128	PERCENT	
CARBON BALANCE	93.91282	PERCENT	
MATERIAL BALANCE	93.92270	PERCENT	

CONV. TO 1. KETONE 0.2122 2. BUTENE 0.0511
5-BUTANOL CONVERSION 0.0011

RUN NUMBER 22

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	696.7	MM HG.
REACTION TEMPERATURE	368.2	DEG. CENTG.
REACTION PRESSURE	699.7	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04698	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82150	
INITIAL CONCENTRATION	0.02952	MOLES/LITER

RUN NUMBER 23

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.0	DEG. C.
ATMOSPHERIC PRESSURE	760.0	MM HG.
REACTION TEMPERATURE	268.0	DEG. C.
REACTION PRESSURE	760.0	MM HG.
WT. OF CATALYST	0.8480	GRAMS
NITROGEN FEED	0.0468	L. MIN.
2-BUTANOL FEED	0.1600	G. MIN.
SPACE VELOCITY	1.0240	MIN. PER G.
INSTR.	0.0125	G. PER MIN.
VOLUME CHANGE	0.8180	
INITIAL CONCENTRATION	0.0500	PERCENT

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.284892	9.766551	17.608902
HYDROGEN	0.252557	0.809940	20.293636
METHANE	0.068551	0.041493	0.130651
BUTENE-1	0.421022	0.399694	0.359858
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	24.725750	24.681046	17.291213
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	62.932204	64.068109	43.662004
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.315022	0.233163	0.653732
TOTAL	100.000000	99.999999	100.000000

MATERIAL BALANCE	96.938093	PERCENT
CARBON BALANCE	96.705141	PERCENT
HYDROGEN BALANCE	97.775289	PERCENT
OXYGEN BALANCE	97.116912	PERCENT

2-BUTANOL CONVERSION 0.31171
 CONV. TO 1. KETONE 0.27257 2. BUTENES 0.00567

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	16.843608	
HYDROGEN	19.411661	0.300978
METHANE	0.124973	0.001937
BUTENE-1	0.478124	0.007413
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.012428	0.000192
METHYL ETHYL KETONE	17.216585	0.266943
1-PROPANOL	0.051657	0.000800
SEC-BUTANOL	45.160821	0.700220
DIETHYL KETONE	0.023966	0.000371
WATER	0.676173	0.010484
TOTAL	100.000000	

MATERIAL BALANCE	97.428882	PERCENT
CARBON BALANCE	97.612684	PERCENT
HYDROGEN BALANCE	98.378575	PERCENT
OXYGEN BALANCE	97.882051	PERCENT

2-BUTANOL CONVERSION 0.29977
 CONV. TO 1. KETONE 0.26694 2. BUTENES 0.00741

COMMENTS: 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 11. 12. 13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24. 25. 26. 27. 28. 29. 30. 31. 32. 33. 34. 35. 36. 37. 38. 39. 40. 41. 42. 43. 44. 45. 46. 47. 48. 49. 50. 51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 69. 70. 71. 72. 73. 74. 75. 76. 77. 78. 79. 80. 81. 82. 83. 84. 85. 86. 87. 88. 89. 90. 91. 92. 93. 94. 95. 96. 97. 98. 99. 100.

WATER	0.31625	0.31625	0.31625
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
I-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000

OXYGEN BALANCE	97.11615	PERCENT
HYDROGEN BALANCE	97.75288	PERCENT
CARBON BALANCE	98.70241	PERCENT
MATERIAL BALANCE	98.08085	PERCENT

CONV. TO 1. KETONE 0.31625 2. BUTENE 0.00000 3-BUTANOL CONVERSION 0.31625

CONVERSIONAL SYSTEM

WATER	0.31625	0.31625	0.31625
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
I-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000

OXYGEN BALANCE	97.11615	PERCENT
HYDROGEN BALANCE	97.75288	PERCENT
CARBON BALANCE	98.70241	PERCENT
MATERIAL BALANCE	98.08085	PERCENT

CONV. TO 1. KETONE 0.31625 2. BUTENE 0.00000 3-BUTANOL CONVERSION 0.31625

RUN NUMBER 23

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.0	DEG. CENTG.
ATMOPHERIC PRESSURE	696.2	MM HG.
REACTION TEMPERATURE	366.7	DEG. CENTG.
REACTION PRESSURE	698.2	MM HG.
WT. OF CATALYST	6.85680	GRAM.
NITROGEN FEED	0.04723	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.02468	MOL/HR.G
1/S.V.	40.51275	G.HR./MOL
VOLUME CHANGE	0.82090	
INITIAL CONCENTRATION	0.02957	MOLES/LITER

Run number 52

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.0	deg. C.
ATMOSPHERIC PRESSURE	760.2	mm. Hg.
REACTION TEMPERATURE	211.7	deg. C.
REACTION PRESSURE	698.3	mm. Hg.
WT. OF CATALYST	6.8550	grams.
NITROGEN FEED	0.0473	g. min.
2-BUTANOL FEED	0.1652	g. min.
SPACE VELOCITY	0.0248	min./vol.
INSTR.	0.0152	g. min.
VOLUME CHANGE	0.0100	
INITIAL CONCENTRATION	0.0262	mol/liter

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.170390	9.670818	17.774147
HYDROGEN	0.229446	0.736081	18.800396
METHANE	0.077805	0.047110	0.151214
BUTENE-1	0.414181	0.393337	0.360996
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	24.942168	24.905732	17.786713
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	62.685063	63.838703	44.348640
DI-ETHYL KETONE	0.161936	0.172021	0.102827
WATER	0.319007	0.236194	0.675062
TOTAL	099.999999	99.999999	100.000000

MATERIAL BALANCE	98.520091	PERCENT
CARBON BALANCE	98.380608	PERCENT
HYDROGEN BALANCE	98.792773	PERCENT
OXYGEN BALANCE	98.773980	PERCENT

2-BUTANOL CONVERSION 0.30372
 CONV. TO 1. KETONE 0.27925 2. BUTENES 0.00566

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	16.447921	
HYDROGEN	17.397596	0.258551
METHANE	0.139931	0.002079
BUTENE-1	0.476435	0.007080
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.006815	0.000101
METHYL ETHYL KETONE	17.466120	0.259570
1-PROPANOL	0.076040	0.001130
SEC-BUTANOL	47.261683	0.702372
DIETHYL KETONE	0.008050	0.000119
WATER	0.719403	0.010691
TOTAL	100.000000	

MATERIAL BALANCE	96.226830	PERCENT
CARBON BALANCE	97.054069	PERCENT
HYDROGEN BALANCE	97.139772	PERCENT
OXYGEN BALANCE	97.388423	PERCENT

2-BUTANOL CONVERSION 0.29762
 CONV. TO 1. KETONE 0.25957 2. BUTENES 0.00708

COMBUSTION ANALYSIS - C-1000

COMPONENT	WGT. PERCENT	WGT. PERCENT	WGT. PERCENT
WATER	0.2100	0.2100	0.2100
DIETHYL KETONE	0.1010	0.1010	0.1010
SEC-BUTANOL	0.2500	0.2500	0.2500
1-PROPANOL	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	0.0000	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000
BUTENE-1	0.0000	0.0000	0.0000
METHANE	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000
NITROGEN	0.0000	0.0000	0.0000
TOTAL	0.0000	0.0000	0.0000

OXYGEN BALANCE	98.7388	PERCENT
HYDROGEN BALANCE	98.7377	PERCENT
CARBON BALANCE	98.3808	PERCENT
MATERIAL BALANCE	98.2000	PERCENT

CONV. TO 1. KETONE 0.2100 2. BUTENE 0.0000 3. BUTENE 0.0000

COMBUSTION ANALYSIS - C-1000

COMPONENT	WGT. PERCENT	WGT. PERCENT	WGT. PERCENT
WATER	0.1100	0.1100	0.1100
DIETHYL KETONE	0.0000	0.0000	0.0000
SEC-BUTANOL	0.2500	0.2500	0.2500
1-PROPANOL	0.0000	0.0000	0.0000
METHYL ETHYL KETONE	0.0000	0.0000	0.0000
UNKNOWN-1	0.0000	0.0000	0.0000
CIS-BUTENE-2	0.0000	0.0000	0.0000
TRANS-BUTENE-2	0.0000	0.0000	0.0000
BUTENE-1	0.0000	0.0000	0.0000
METHANE	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000
NITROGEN	0.0000	0.0000	0.0000
TOTAL	0.0000	0.0000	0.0000

OXYGEN BALANCE	97.2822	PERCENT
HYDROGEN BALANCE	97.1302	PERCENT
CARBON BALANCE	97.0000	PERCENT
MATERIAL BALANCE	96.2280	PERCENT

CONV. TO 1. KETONE 0.2100 2. BUTENE 0.0000 3. BUTENE 0.0000

RUN NUMBER 24

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	700.4	MM HG.
REACTION TEMPERATURE	347.6	DEG. CENTG.
REACTION PRESSURE	703.4	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04747	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.05000	MOL/HR.G
1/S.V.	19.99699	G.HR./MOL
VOLUME CHANGE	0.82029	
INITIAL CONCENTRATION	0.02961	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	deg. C.
ATMOSPHERIC PRESSURE	700.4	mm. Hg.
REACTION TEMPERATURE	347.8	deg. C.
REACTION PRESSURE	703.4	mm. Hg.
WT. OF CATALYST	3.3850	GRAMS
NITROGEN FEED	0.0474	g. MINUTE
2-BUTANOL FEED	0.1850	g. MINUTE
SPACE VELOCITY	0.0000	MINUTE
INLET V.	10.0000	MINUTE
VOLUME CHANGE	0.0000	
INITIAL CONCENTRATION	0.0000	

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.208891	9.696367	20.100465
HYDROGEN	0.095393	0.305785	8.809057
METHANE	0.006603	0.003994	0.014462
BUTENE-1	0.122176	0.115935	0.120011
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	10.151210	10.128251	8.158351
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	78.141995	79.516275	62.305127
DI-ETHYL KETONE	0.096021	0.101920	0.068715
WATER	0.177706	0.131469	0.423808
TOTAL	100.000000	100.000000	100.000000

MATERIAL BALANCE	98.749722	PERCENT
CARBON BALANCE	98.631681	PERCENT
HYDROGEN BALANCE	98.877156	PERCENT
OXYGEN BALANCE	99.026641	PERCENT

2-BUTANOL CONVERSION 0.13046
 CONV. TO 1. KETONE 0.11385 2. BUTENES 0.00167

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	23.050088	
HYDROGEN	10.101733	0.149699
METHANE	0.016585	0.000245
BUTENE-1	0.193858	0.002872
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.001232	0.000018
METHYL ETHYL KETONE	6.974461	0.103355
1-PROPANOL	0.030124	0.000446
SEC-BUTANOL	59.228879	0.877724
DIETHYL KETONE	0.000152	0.000002
WATER	0.402883	0.005970
TOTAL	099.999999	

MATERIAL BALANCE	100.850985	PERCENT
CARBON BALANCE	98.435269	PERCENT
HYDROGEN BALANCE	99.429957	PERCENT
OXYGEN BALANCE	98.749988	PERCENT

2-BUTANOL CONVERSION 0.12227
 CONV. TO 1. KETONE 0.10335 2. BUTENES 0.00287

COMPARISON OF MATERIAL BALANCE

COMPONENT		MATERIAL BALANCE		HYDROGEN BALANCE		OXYGEN BALANCE	
NITROGEN		11.0000		99.9999		99.9999	
HYDROGEN		11.0000		99.9999		99.9999	
METHANE		0.0000		0.0000		0.0000	
BUTENE-1		0.0000		0.0000		0.0000	
TRANS-BUTENE-2		0.0000		0.0000		0.0000	
CIS-BUTENE-2		0.0000		0.0000		0.0000	
UNKNOWN-1		0.0000		0.0000		0.0000	
METHYL ETHYL KETONE		10.0000		99.9999		99.9999	
I-PROPANOL		0.0000		0.0000		0.0000	
SEC-BUTANOL		18.0000		99.9999		99.9999	
DIETHYL KETONE		0.0000		0.0000		0.0000	
WATER		0.0000		0.0000		0.0000	
TOTAL		100.0000		100.0000		100.0000	
MATERIAL BALANCE		99.9999		99.9999		99.9999	
CARBON BALANCE		99.9999		99.9999		99.9999	
HYDROGEN BALANCE		99.9999		99.9999		99.9999	
OXYGEN BALANCE		99.9999		99.9999		99.9999	
S-BUTANOL CONVERSION		0.0000		0.0000		0.0000	
CONV. TO I. KETONE		0.0000		0.0000		0.0000	

COMPARISON OF MATERIAL BALANCE

COMPONENT		MATERIAL BALANCE		HYDROGEN BALANCE		OXYGEN BALANCE	
NITROGEN		11.0000		99.9999		99.9999	
HYDROGEN		11.0000		99.9999		99.9999	
METHANE		0.0000		0.0000		0.0000	
BUTENE-1		0.0000		0.0000		0.0000	
TRANS-BUTENE-2		0.0000		0.0000		0.0000	
CIS-BUTENE-2		0.0000		0.0000		0.0000	
UNKNOWN-1		0.0000		0.0000		0.0000	
METHYL ETHYL KETONE		10.0000		99.9999		99.9999	
I-PROPANOL		0.0000		0.0000		0.0000	
SEC-BUTANOL		18.0000		99.9999		99.9999	
DIETHYL KETONE		0.0000		0.0000		0.0000	
WATER		0.0000		0.0000		0.0000	
TOTAL		100.0000		100.0000		100.0000	
MATERIAL BALANCE		99.9999		99.9999		99.9999	
CARBON BALANCE		99.9999		99.9999		99.9999	
HYDROGEN BALANCE		99.9999		99.9999		99.9999	
OXYGEN BALANCE		99.9999		99.9999		99.9999	
S-BUTANOL CONVERSION		0.0000		0.0000		0.0000	
CONV. TO I. KETONE		0.0000		0.0000		0.0000	

RUN NUMBER 25

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.2	DEG. CENTG.
ATMOPHERIC PRESSURE	701.4	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENTG.
REACTION PRESSURE	704.4	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04474	G. MOL/HR
2-BUTANOL FEED	0.12719	G. MOL/HR
SPACE VELOCITY	0.03758	MOL/HR.G
1/S.V.	26.60923	G.HR./MOL
VOLUME CHANGE	0.79350	
INITIAL CONCENTRATION	0.02817	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.2 DEG. CELSI.
ATMOSPHERIC PRESSURE	701.4 MM. HG.
REACTION TEMPERATURE	240.0 DEG. CELSI.
REACTION PRESSURE	704.4 MM. HG.
WT. OF CATALYST	3.38450 GRAMS
NITROGEN FEED	0.04474 G. MIN.
2-BUTANOL FEED	0.12514 G. MIN.
SPACE VELOCITY	0.03758 MIN. ⁻¹
INSTR.	56.80253 G. MIN.
VOLUME CHANGE	0.10320
INITIAL CONCENTRATION	0.02917 MOL/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	13.504136	11.728181	23.820888
HYDROGEN	0.088446	0.284637	8.034062
METHANE	0.011585	0.007036	0.024960
BUTENE-1	0.121612	0.115856	0.117505
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	11.433086	11.452428	9.038487
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	74.665606	76.279804	58.560878
DI-ETHYL KETONE	0.005212	0.005554	0.003669
WATER	0.170315	0.126500	0.399547
TOTAL	099.999999	100.000000	100.000000

MATERIAL BALANCE	100.077846	PERCENT
CARBON BALANCE	100.019384	PERCENT
HYDROGEN BALANCE	99.810198	PERCENT
OXYGEN BALANCE	100.425329	PERCENT

2-BUTANOL CONVERSION 0.13518
 CONV. TO 1. KETONE 0.13347 2. BUTENES 0.00173

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	22.617105	
HYDROGEN	7.628063	0.107120
METHANE	0.023699	0.000332
BUTENE-1	0.165852	0.002329
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	8.183690	0.114923
1-PROPANOL	0.000000	0.000000
SEC-BUTANOL	60.965231	0.856131
DIETHYL KETONE	0.000405	0.000005
WATER	0.415951	0.005841
TOTAL	099.999999	

MATERIAL BALANCE	96.567535	PERCENT
CARBON BALANCE	97.347430	PERCENT
HYDROGEN BALANCE	97.266469	PERCENT
OXYGEN BALANCE	97.690180	PERCENT

2-BUTANOL CONVERSION 0.14386
 CONV. TO 1. KETONE 0.11492 2. BUTENES 0.00232

GROUP 2: REACTION 2: 1.1.1.1

COMPONENT	WGT. PERCENT	WGT. PERCENT	WGT. PERCENT
WATER	0.17032	0.17032	0.17032
DIETHYL KETONE	0.00212	0.00212	0.00212
SEC-BUTANOL	24.66240	24.66240	24.66240
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	11.42102	11.42102	11.42102
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.12102	0.12102	0.12102
METHANE	0.01102	0.01102	0.01102
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000

OXYGEN BALANCE	100.45224	PERCENT
HYDROGEN BALANCE	99.81018	PERCENT
CARBON BALANCE	100.07234	PERCENT
MATERIAL BALANCE	100.07234	PERCENT

CONV. TO 1. KETONE 0.13247 2. BUTENES 0.00129
2-BUTANOL CONVERSION 0.13247

CONVENTIONAL SYSTEM

COMPONENT	WGT. PERCENT	WGT. PERCENT
WATER	0.17032	0.17032
DIETHYL KETONE	0.00212	0.00212
SEC-BUTANOL	24.66240	24.66240
1-PROPANOL	0.00000	0.00000
METHYL ETHYL KETONE	11.42102	11.42102
UNKNOWN-1	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000
BUTENE-1	0.12102	0.12102
METHANE	0.01102	0.01102
HYDROGEN	0.00000	0.00000
NITROGEN	0.00000	0.00000
TOTAL	100.00000	100.00000

OXYGEN BALANCE	97.80100	PERCENT
HYDROGEN BALANCE	97.26463	PERCENT
CARBON BALANCE	97.34230	PERCENT
MATERIAL BALANCE	97.26233	PERCENT

CONV. TO 1. KETONE 0.11023 2. BUTENES 0.00043
2-BUTANOL CONVERSION 0.11023

RUN NUMBER 26

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	700.2	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENTG.
REACTION PRESSURE	702.2	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04549	G. MOL/HR
2-BUTANOL FEED	0.08468	G. MOL/HR
SPACE VELOCITY	0.02502	MOL/HR.G
1/S.V.	39.96659	G.HR./MOL
VOLUME CHANGE	0.74103	
INITIAL CONCENTRATION	0.02466	MOLES/LITER

INITIAL CONCENTRATION	VOLUME CHANGE	1/2 V.	SPACE VELOCITY	2-BUTANOL FEED	NITROGEN FEED	WT. OF CATALYST	REACTION PRESSURE	REACTION TEMPERATURE	ATMOSPHERIC PRESSURE	ROOM TEMPERATURE
0.0246	0.74103	89.8829	0.02702	0.0848	0.0424	3.32420	705.5	349.0	710.5	53.0
0.0246	0.74103	89.8829	0.02702	0.0848	0.0424	3.32420	705.5	349.0	710.5	53.0

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	19.593155	17.173551	32.008970
HYDROGEN	0.110302	0.358253	9.279352
METHANE	0.015083	0.009246	0.030098
BUTENE-1	0.165869	0.159478	0.148431
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.011046	0.008554	0.009710
METHYL ETHYL KETONE	12.713676	12.852782	9.308497
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	67.001075	69.081639	48.668162
DI-ETHYL KETONE	0.197342	0.212235	0.128656
WATER	0.192447	0.144258	0.418120
TOTAL	99.999999	99.999999	100.000000
MATERIAL BALANCE	97.926166	PERCENT	
CARBON BALANCE	97.828875	PERCENT	
HYDROGEN BALANCE	97.863210	PERCENT	
OXYGEN BALANCE	98.214866	PERCENT	

2-BUTANOL CONVERSION 0.18324
 CONV. TO 1. KETONE 0.15621 2. BUTENES 0.00249

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	30.642590	
HYDROGEN	8.883240	0.143331
METHANE	0.028813	0.000464
BUTENE-1	0.187479	0.003024
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.019614	0.000316
METHYL ETHYL KETONE	8.785969	0.141761
1-PROPANOL	0.061038	0.000984
SEC-BUTANOL	50.928716	0.821736
DIETHYL KETONE	0.024996	0.000403
WATER	0.437541	0.007059
TOTAL	100.000000	
MATERIAL BALANCE	96.079561	PERCENT
CARBON BALANCE	96.788288	PERCENT
HYDROGEN BALANCE	96.902188	PERCENT
OXYGEN BALANCE	97.194681	PERCENT

2-BUTANOL CONVERSION 0.17826
 CONV. TO 1. KETONE 0.14176 2. BUTENES 0.00302

COMPARISON OF MATERIAL BALANCE

COMPONENT	PERCENT	PERCENT	PERCENT
WATER	0.18247	0.14458	0.01481
DIETHYL KETONE	0.17345	0.51555	0.17250
SEC-BUTANOL	0.00105	0.00139	0.00034
I-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	12.71574	12.56570	0.00000
UNKNOWN-1	0.00104	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.16400	0.15475	0.00000
METANE	0.00000	0.00000	0.00000
HYDROGEN	0.11675	0.11675	0.00000
WATER	0.18247	0.14458	0.01481
TOTAL	99.99999	99.99999	100.00000
OXYGEN BALANCE	99.51886	PERCENT	
HYDROGEN BALANCE	97.86310	PERCENT	
CARBON BALANCE	97.82875	PERCENT	
MATERIAL BALANCE	97.02816	PERCENT	
CONV. TO 1. KETONE 0.18247			
2-BUTANOL CONVERSION	0.18247		

COMPARISON OF MATERIAL BALANCE

COMPONENT	PERCENT	PERCENT	PERCENT
WATER	0.43751	0.02998	0.00000
DIETHYL KETONE	0.02998	0.02998	0.00000
SEC-BUTANOL	20.02714	0.00000	0.00000
I-PROPANOL	0.00108	0.00000	0.00000
METHYL ETHYL KETONE	8.78605	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.10747	0.00000	0.00000
METHANE	0.028813	0.00000	0.00000
HYDROGEN	8.88240	0.14814	0.00000
NITROGEN	30.44250	0.14814	0.00000
TOTAL	100.00000		
OXYGEN BALANCE	97.10491	PERCENT	
HYDROGEN BALANCE	98.00218	PERCENT	
CARBON BALANCE	99.78028	PERCENT	
MATERIAL BALANCE	99.07951	PERCENT	
CONV. TO 1. KETONE 0.18247			
2-BUTANOL CONVERSION	0.18247		

RUN NUMBER 27

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENTG.
ATMOPHERIC PRESSURE	700.3	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENTG.
REACTION PRESSURE	707.3	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04225	G. MOL/HR
2-BUTANOL FEED	0.34432	G. MOL/HR
SPACE VELOCITY	0.10173	MOL/HR.G
1/S.V.	9.82939	G.HR./MOL
VOLUME CHANGE	0.90145	
INITIAL CONCENTRATION	0.03377	MOLES/LITER

TABLE 1

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	23.0	DEG. CENT.
ATMOSPHERIC PRESSURE	700.3	MM. HG.
REACTION TEMPERATURE	340.0	DEG. CENT.
REACTION PRESSURE	707.3	MM. HG.
WT. OF CATALYST	2.8450	GRAMS.
NITROGEN FEED	0.0452	G. PER HOUR
S-BUTANOL FEED	0.3443	G. PER HOUR
SPACE VELOCITY	0.1013	PER HOUR
INSTR.	0.0239	G. PER HOUR
VOLUME CHANGE	0.0145	
INITIAL CONCENTRATION	0.0335	MOLES PER LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	5.125118	4.392448	10.148139
HYDROGEN	0.059276	0.188249	6.044069
METHANE	0.002964	0.001777	0.007170
BUTENE-1	0.047274	0.044443	0.051274
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	6.677080	6.600239	5.925299
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	87.621653	88.336335	77.141810
DI-ETHYL KETONE	0.296535	0.311833	0.234316
WATER	0.170095	0.124672	0.447918
TOTAL	099.999999	100.000000	099.999999

MATERIAL BALANCE	100.972420	PERCENT
CARBON BALANCE	100.877484	PERCENT
HYDROGEN BALANCE	100.932607	PERCENT
OXYGEN BALANCE	101.284163	PERCENT

2-BUTANOL CONVERSION 0.06706
 CONV. TO 1. KETONE 0.07165 2. BUTENES 0.00062

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	10.735196	
HYDROGEN	6.393711	0.075106
METHANE	0.007585	0.000089
BUTENE-1	0.113339	0.001331
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.002700	0.000031
METHYL ETHYL KETONE	5.374213	0.063130
1-PROPANOL	0.024206	0.000284
SEC-BUTANOL	76.845606	0.902699
DIETHYL KETONE	0.057241	0.000672
WATER	0.446199	0.005241
TOTAL	099.999999	

MATERIAL BALANCE	97.203409	PERCENT
CARBON BALANCE	96.823731	PERCENT
HYDROGEN BALANCE	97.127400	PERCENT
OXYGEN BALANCE	97.202809	PERCENT

2-BUTANOL CONVERSION 0.09730
 CONV. TO 1. KETONE 0.06313 2. BUTENES 0.00133

COMPOSITIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
NITROGEN	0.12519	0.12519	0.12519
HYDROGEN	0.02272	0.02272	0.02272
METHANE	0.00000	0.00000	0.00000
BUTENE-1	0.04737	0.04737	0.04737
TRANS-BUTENE-2	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
I-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
DI-ETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.12000	0.12000	0.12000
TOTAL	0.99999	100.00000	0.99999
OXYGEN BALANCE	101.20413	PERCENT	
HYDROGEN BALANCE	100.92507	PERCENT	
CARBON BALANCE	100.07444	PERCENT	
MATERIAL BALANCE	100.07444	PERCENT	
CONV. TO I. KETONE 0.0012	0.0012		
2-BUTANOL CONVERSION	0.0012		

COMPOSITIONAL SYSTEM

COMPONENT	WGT PERCENT	WGT PERCENT	WGT PERCENT
NITROGEN	0.12519	0.12519	0.12519
HYDROGEN	0.02272	0.02272	0.02272
METHANE	0.00000	0.00000	0.00000
BUTENE-1	0.11338	0.11338	0.11338
TRANS-BUTENE-2	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
I-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
DI-ETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.00000	0.00000	0.00000
TOTAL	0.99999	100.00000	0.99999
OXYGEN BALANCE	97.20800	PERCENT	
HYDROGEN BALANCE	97.12400	PERCENT	
CARBON BALANCE	96.82331	PERCENT	
MATERIAL BALANCE	97.20800	PERCENT	
CONV. TO I. KETONE 0.0012	0.0012		
2-BUTANOL CONVERSION	0.0012		

RUN NUMBER 28

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.8	DEG. CENTG.
ATMOPHERIC PRESSURE	700.5	MM HG.
REACTION TEMPERATURE	348.8	DEG. CENTG.
REACTION PRESSURE	705.5	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04474	G. MOL/HR
2-BUTANOL FEED	0.25421	G. MOL/HR
SPACE VELOCITY	0.07511	MOL/HR.G
1/S.V.	13.31340	G.HR./MOL
VOLUME CHANGE	0.86981	
INITIAL CONCENTRATION	0.03227	MOLES/LITER

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.8 DEG. C.
ATMOSPHERIC PRESSURE	760.2 MM. HG.
REACTION TEMPERATURE	348.8 DEG. C.
REACTION PRESSURE	702.2 MM. HG.
WT. OF CATALYST	3.38450 GRAM.
NITROGEN FEED	0.04474 G. MIN.
2-BUTANOL FEED	0.52451 G. MIN.
SPACE VELOCITY	0.07511 MIN. ⁻¹
INLET V.	13.31340 G. MIN.
VOLUME CHANGE	0.06981
INITIAL CONCENTRATION	0.03552

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	7.198949	6.189376	13.768251
HYDROGEN	0.070237	0.223767	6.917420
METHANE	0.006376	0.003834	0.014896
BUTENE-1	0.067898	0.064035	0.071131
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	6.823621	6.766482	5.848785
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	85.289914	86.258233	72.527577
DI-ETHYL KETONE	0.297250	0.313575	0.226869
WATER	0.245750	0.180695	0.625067
TOTAL	100.000000	99.999999	100.000000

MATERIAL BALANCE	100.834306	PERCENT
CARBON BALANCE	100.651543	PERCENT
HYDROGEN BALANCE	100.996741	PERCENT
OXYGEN BALANCE	101.282407	PERCENT

2-BUTANOL CONVERSION 0.07283
 CONV. TO 1. KETONE 0.07476 2. BUTENES 0.00090

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	13.026647	
HYDROGEN	6.544825	0.077624
METHANE	0.014094	0.000167
BUTENE-1	0.141863	0.001682
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	6.360972	0.075444
1-PROPANOL	0.012388	0.000146
SEC-BUTANOL	73.221524	0.868443
DIETHYL KETONE	0.046635	0.000553
WATER	0.631048	0.007484
TOTAL	099.999999	

MATERIAL BALANCE	94.049911	PERCENT
CARBON BALANCE	94.641335	PERCENT
HYDROGEN BALANCE	94.790400	PERCENT
OXYGEN BALANCE	95.207198	PERCENT

2-BUTANOL CONVERSION 0.13155
 CONV. TO 1. KETONE 0.07544 2. BUTENES 0.00168

COMPARISON OF THE TWO SYSTEMS

COMPONENT	WATER	WATER	WATER
WATER	0.24250	0.18082	0.24250
DIETHYL KETONE	0.29250	0.31322	0.29250
SEC-BUTANOL	0.29250	0.29250	0.29250
I-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	99.99999	100.00000
OXYGEN BALANCE	101.28207	PERCENT	
HYDROGEN BALANCE	100.99142	PERCENT	
CARBON BALANCE	100.88406	PERCENT	
MATERIAL BALANCE	100.88406	PERCENT	

CONV. TO I. KETONE 0.004% 2. BUTENE 0.004%
2-BUTANOL CONVERSION 0.00283

CONVENTIONAL SYSTEM

COMPONENT	WATER	WATER	WATER
WATER	0.24250	0.18082	0.24250
DIETHYL KETONE	0.29250	0.31322	0.29250
SEC-BUTANOL	0.29250	0.29250	0.29250
I-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	99.99999	100.00000
OXYGEN BALANCE	101.28207	PERCENT	
HYDROGEN BALANCE	100.99142	PERCENT	
CARBON BALANCE	100.88406	PERCENT	
MATERIAL BALANCE	100.88406	PERCENT	

CONV. TO I. KETONE 0.004% 2. BUTENE 0.004%
2-BUTANOL CONVERSION 0.00283

RUN NUMBER 29

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.2	DEG. CENTG.
ATMOPHERIC PRESSURE	697.5	MM HG.
REACTION TEMPERATURE	350.0	DEG. CENTG.
REACTION PRESSURE	700.5	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04524	G. MOL/HR
2-BUTANOL FEED	0.25421	G. MOL/HR
SPACE VELOCITY	0.07511	MOL/HR.G
1/S.V.	13.31340	G.HR./MOL
VOLUME CHANGE	0.86875	
INITIAL CONCENTRATION	0.03214	MOLES/LITER

WILL NUMBER 29

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.5 DEC. C.WTG.
ATMOSPHERIC PRESSURE	737.5 IN. HG.
REACTION TEMPERATURE	280.0 DEC. C.WTG.
REACTION PRESSURE	700.5 IN. HG.
WT. OF CATALYST	3.38450 GRAM.
NITROGEN FEED	0.04254 C. MOL/LHR.
S-BUTANE FEED	0.52451 C. MOL/LHR.
SPACE VELOCITY	0.07511 MOL/LHR.G.
152.V.	13.31840 C. HR./VOL.
VOLUME CHANGE	0.00885
INITIAL CONCENTRATION	0.03314 MOLES/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	7.314192	6.290959	14.238421
HYDROGEN	0.052078	0.165980	5.220576
METHANE	0.013221	0.007953	0.031437
BUTENE-1	0.061795	0.058302	0.065893
TRANS-BUTENE-2	0.004865	0.004333	0.004897
CIS-BUTENE-2	0.003495	0.003043	0.003439
UNKNOWN-1	0.004083	0.003103	0.004277
METHYL ETHYL KETONE	6.629548	6.576649	5.783896
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	85.460682	86.465319	73.970341
DI-ETHYL KETONE	0.278036	0.293423	0.215993
WATER	0.177998	0.130931	0.460824
TOTAL	100.000000	100.000000	100.000000

MATERIAL BALANCE	100.199755	PERCENT
CARBON BALANCE	100.123560	PERCENT
HYDROGEN BALANCE	100.017784	PERCENT
OXYGEN BALANCE	100.529441	PERCENT

2-BUTANOL CONVERSION 0.07545
 CONV. TO 1. KETONE 0.07229 2. BUTENES 0.00092

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	14.560679	
HYDROGEN	5.338733	0.065442
METHANE	0.032149	0.000394
BUTENE-1	0.113565	0.001392
TRANS BUTENE-2	0.005244	0.000064
CIS BUTENE-2	0.003748	0.000045
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	5.159311	0.063242
1-PROPANOL	0.011031	0.000135
SEC-BUTANOL	74.280590	0.910531
DIETHYL KETONE	0.032189	0.000394
WATER	0.462757	0.005672
TOTAL	100.000000	

MATERIAL BALANCE	97.623278	PERCENT
CARBON BALANCE	97.596951	PERCENT
HYDROGEN BALANCE	97.721064	PERCENT
OXYGEN BALANCE	97.997631	PERCENT

2-BUTANOL CONVERSION 0.08946
 CONV. TO 1. KETONE 0.06324 2. BUTENES 0.00150

CONVENTIONAL SYSTEM

COMPONENT			MATERIAL BALANCE		
PERCENT			PERCENT		
WATER	0.17098	0.17098	WATER	0.17098	0.17098
DIETHYL KETONE	0.27036	0.27036	DIETHYL KETONE	0.27036	0.27036
SEC-BUTANOL	0.48065	0.48065	SEC-BUTANOL	0.48065	0.48065
1-PROPANOL	0.00000	0.00000	1-PROPANOL	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	METHYL ETHYL KETONE	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	UNKNOWN-1	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	CIS-BUTENE-2	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	TRANS-BUTENE-2	0.00000	0.00000
BUTENE-1	0.00000	0.00000	BUTENE-1	0.00000	0.00000
METHANE	0.00000	0.00000	METHANE	0.00000	0.00000
HYDROGEN	0.00000	0.00000	HYDROGEN	0.00000	0.00000
NITROGEN	0.00000	0.00000	NITROGEN	0.00000	0.00000
TOTAL			TOTAL		
100.00000			100.00000		

CONV. TO 1. KETONE 0.00000 2. BUTENE 0.00000
S-BUTANOL CONVERSION 0.00000

CONVENTIONAL SYSTEM

COMPONENT			MATERIAL BALANCE		
PERCENT			PERCENT		
WATER	0.45383	0.45383	WATER	0.45383	0.45383
DIETHYL KETONE	0.03188	0.03188	DIETHYL KETONE	0.03188	0.03188
SEC-BUTANOL	0.28050	0.28050	SEC-BUTANOL	0.28050	0.28050
1-PROPANOL	0.11031	0.11031	1-PROPANOL	0.11031	0.11031
METHYL ETHYL KETONE	0.15911	0.15911	METHYL ETHYL KETONE	0.15911	0.15911
UNKNOWN-1	0.00000	0.00000	UNKNOWN-1	0.00000	0.00000
CIS BUTENE-2	0.00378	0.00378	CIS BUTENE-2	0.00378	0.00378
TRANS BUTENE-2	0.00264	0.00264	TRANS BUTENE-2	0.00264	0.00264
BUTENE-1	0.11388	0.11388	BUTENE-1	0.11388	0.11388
METHANE	0.00000	0.00000	METHANE	0.00000	0.00000
HYDROGEN	0.38833	0.38833	HYDROGEN	0.38833	0.38833
NITROGEN	0.00000	0.00000	NITROGEN	0.00000	0.00000
TOTAL			TOTAL		
100.00000			100.00000		

CONV. TO 1. KETONE 0.00000 2. BUTENE 0.00000
S-BUTANOL CONVERSION 0.00000

RUN NUMBER 30

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.3	DEG. CENTG.
ATMOPHERIC PRESSURE	697.5	MM HG.
REACTION TEMPERATURE	349.5	DEG. CENTG.
REACTION PRESSURE	700.5	MM HG.
WT. OF CATALYST	3.38450	GRAM.
NITROGEN FEED	0.04598	G. MOL/HR
2-BUTANOL FEED	0.12719	G. MOL/HR
SPACE VELOCITY	0.03758	MOL/HR.G
1/S.V.	26.60923	G.HR./MOL
VOLUME CHANGE	0.79017	
INITIAL CONCENTRATION	0.02780	MOLES/LITER

WMA NUMBER: 30

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.3	DEG. CENT.
ATMOSPHERIC PRESSURE	697.2	MM. HG.
REACTION TEMPERATURE	344.2	DEG. CENT.
REACTION PRESSURE	700.2	MM. HG.
WT. OF CATALYST	2.8820	GRAM.
NITROGEN FEED	0.04608	L. PER HOUR
S-BUTANOL FEED	0.12319	L. PER HOUR
SPACE VELOCITY	0.03720	PER HOUR
INLET V.	26.8023	G. PER HOUR
VOLUME CHANGE	0.2901	
INITIAL CONCENTRATION	0.05380	PERCENT

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	13.943207	12.119745	24.817329
HYDROGEN	0.073001	0.235133	6.690998
METHANE	0.020384	0.012392	0.044316
BUTENE-1	0.122993	0.117271	0.119913
TRANS-BUTENE-2	0.001895	0.001706	0.001744
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.008319	0.006388	0.007967
METHYL ETHYL KETONE	9.717401	9.742068	7.751461
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	75.901053	77.607508	60.067008
DI-ETHYL KETONE	0.001179	0.001258	0.000837
WATER	0.210563	0.156526	0.498422
TOTAL	099.999999	099.999999	100.000000

MATERIAL BALANCE	99.093134	PERCENT
CARBON BALANCE	98.997418	PERCENT
HYDROGEN BALANCE	98.807586	PERCENT
OXYGEN BALANCE	99.529868	PERCENT

2-BUTANOL CONVERSION 0.12490
 CONV. TO 1. KETONE 0.11292 2. BUTENES 0.00177

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	24.067259	
HYDROGEN	6.488772	0.091019
METHANE	0.042976	0.000602
BUTENE-1	0.158833	0.002227
TRANS BUTENE-2	0.002268	0.000031
CIS BUTENE-2	0.010331	0.000144
UNKNOWN-1	0.000000	0.000000
METHYL ETHYL KETONE	7.634499	0.107090
1-PROPANOL	0.042630	0.000597
SEC-BUTANOL	61.006316	0.855748
DIETHYL KETONE	0.039893	0.000559
WATER	0.506216	0.007100
TOTAL	100.000000	

MATERIAL BALANCE	96.312096	PERCENT
CARBON BALANCE	96.654311	PERCENT
HYDROGEN BALANCE	96.424848	PERCENT
OXYGEN BALANCE	97.109807	PERCENT

2-BUTANOL CONVERSION 0.14425
 CONV. TO 1. KETONE 0.10709 2. BUTENES 0.00240

COMPOSITIONAL ANALYSIS

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
WATER	0.21053	0.15253	0.15253
DIETHYL KETONE	0.00179	0.00179	0.00179
SEC-BUTANOL	25.90153	25.90153	25.90153
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.71491	0.71491	0.71491
UNKNOWN-1	0.00831	0.00831	0.00831
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00195	0.00195	0.00195
BUTENE-1	0.15253	0.15253	0.15253
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	17.96253	17.96253	17.96253

OXYGEN BALANCE	99.52888	PERCENT
HYDROGEN BALANCE	98.80288	PERCENT
CARBON BALANCE	98.99718	PERCENT
MATERIAL BALANCE	99.09334	PERCENT

CONV. TO 1. KETONE 0.11595 2. BUTENES 0.00179
2-BUTANOL CONVERSION 0.15490

COMPOSITIONAL ANALYSIS

COMPONENT	MOLE PERCENT	WT PERCENT	MOLE PERCENT
WATER	0.20216	0.03893	0.03893
DIETHYL KETONE	0.03893	0.03893	0.03893
SEC-BUTANOL	0.00315	0.00315	0.00315
1-PROPANOL	0.00250	0.00250	0.00250
METHYL ETHYL KETONE	3.52449	3.52449	3.52449
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.01033	0.01033	0.01033
TRANS-BUTENE-2	0.00252	0.00252	0.00252
BUTENE-1	0.15883	0.15883	0.15883
METHANE	0.04593	0.04593	0.04593
HYDROGEN	5.48772	5.48772	5.48772
NITROGEN	24.08759	24.08759	24.08759

OXYGEN BALANCE	97.10907	PERCENT
HYDROGEN BALANCE	98.44840	PERCENT
CARBON BALANCE	98.42431	PERCENT
MATERIAL BALANCE	96.31206	PERCENT

CONV. TO 1. KETONE 0.10200 2. BUTENES 0.10200
2-BUTANOL CONVERSION 0.10000

RUN NUMBER 31

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.5	DEG. CENTG.
ATMOPHERIC PRESSURE	695.6	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENTG.
REACTION PRESSURE	698.6	MM HG.
WT. OF CATALYST	5.07740	GRAM.
NITROGEN FEED	0.04598	G. MOL/HR
2-BUTANOL FEED	0.12719	G. MOL/HR
SPACE VELOCITY	0.02505	MOL/HR.G
1/S.V.	39.91897	G.HR./MOL
VOLUME CHANGE	0.79017	
INITIAL CONCENTRATION	0.02770	MOLES/LITER

Run Number: 31

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.5	deg. C.	Water.
ATMOSPHERIC PRESSURE	692.4	mm. Hg.	
REACTION TEMPERATURE	349.0	deg. C.	
REACTION PRESSURE	600.0	mm. Hg.	
WT. OF CATALYST	2.0340	grams	
NITROGEN FEED	0.0498	G. MIN.	
2-BUTANOL FEED	0.1319	G. MIN.	
SPACE VELOCITY	0.0595	MIN./VOL.	
INSTR.	30.9184	P. Hg. Vac.	
VOLUME CHANGE	0.3901		
INITIAL CONCENTRATION	0.0270	MOLES/LITER	

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	13.738484	11.937317	23.536992
HYDROGEN	0.116629	0.375514	10.289305
METHANE	0.012083	0.007343	0.025285
BUTENE-1	0.190174	0.181258	0.178466
TRANS-BUTENE-2	0.009820	0.008836	0.008700
CIS-BUTENE-2	0.012913	0.011358	0.011183
UNKNOWN-1	0.009490	0.007284	0.008747
METHYL ETHYL KETONE	13.139370	13.167785	10.088528
1-PROPANOL	0.000183	0.000180	0.000165
SEC-BUTANOL	72.445839	74.046834	55.185049
DI-ETHYL KETONE	0.045735	0.048760	0.031268
WATER	0.279273	0.207526	0.636305
TOTAL	99.999999	99.999999	100.000000

MATERIAL BALANCE	100.816340	PERCENT
CARBON BALANCE	100.642432	PERCENT
HYDROGEN BALANCE	100.832497	PERCENT
OXYGEN BALANCE	101.293527	PERCENT

2-BUTANOL CONVERSION 0.15229
 CONV. TO 1. KETONE 0.15497 2. BUTENES 0.00304

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	22.644760	
HYDROGEN	9.899262	0.143499
METHANE	0.024327	0.000352
BUTENE-1	0.227871	0.003303
TRANS BUTENE-2	0.008556	0.000124
CIS BUTENE-2	0.011484	0.000166
UNKNOWN-1	0.067328	0.000975
METHYL ETHYL KETONE	10.317948	0.149568
1-PROPANOL	0.052262	0.000757
SEC-BUTANOL	56.062290	0.812677
DIETHYL KETONE	0.037488	0.000543
WATER	0.646420	0.009370
TOTAL	099.999999	

MATERIAL BALANCE	96.159050	PERCENT
CARBON BALANCE	96.717561	PERCENT
HYDROGEN BALANCE	96.707203	PERCENT
OXYGEN BALANCE	97.291776	PERCENT

2-BUTANOL CONVERSION 0.18732
 CONV. TO 1. KETONE 0.14956 2. BUTENES 0.00359

COMPOSITIONAL ANALYSIS OF 2-BUTANOL

COMPONENT	WGT. PERCENT	MOLE PERCENT	WGT. PERCENT
WATER	0.2543	0.2543	0.2543
DIETHYL KETONE	0.0473	0.0473	0.0473
SEC-BUTANOL	12.4488	12.4488	12.4488
1-PROPANOL	0.0018	0.0018	0.0018
METHYL ETHYL KETONE	12.4488	12.4488	12.4488
UNKNOWN-1	0.0040	0.0040	0.0040
CIS-2-BUTENE-2	0.0182	0.0182	0.0182
TRANS-2-BUTENE-2	0.0083	0.0083	0.0083
BUTENE-1	0.1012	0.1012	0.1012
METHANE	0.0123	0.0123	0.0123
UNKNOWN-2	0.1182	0.1182	0.1182
WATER	18.4524	18.4524	18.4524
TOTAL	99.9999	99.9999	100.0000

WATERIAL BALANCE	100.0000
CARBON BALANCE	100.0000
HYDROGEN BALANCE	100.0000
OXYGEN BALANCE	101.2522

CONV. TO 1. KETONE 0.1244 2. BUTENE 0.0083
2-BUTANOL CONVERSION 0.1244

COMPOSITIONAL ANALYSIS OF 2-BUTANOL

COMPONENT	WGT. PERCENT	MOLE PERCENT
WATER	0.2543	0.2543
DIETHYL KETONE	0.0473	0.0473
SEC-BUTANOL	12.4488	12.4488
1-PROPANOL	0.0018	0.0018
METHYL ETHYL KETONE	12.4488	12.4488
UNKNOWN-1	0.0040	0.0040
CIS-2-BUTENE-2	0.0182	0.0182
TRANS-2-BUTENE-2	0.0083	0.0083
BUTENE-1	0.1012	0.1012
METHANE	0.0123	0.0123
UNKNOWN-2	0.1182	0.1182
WATER	18.4524	18.4524
TOTAL	99.9999	99.9999

WATERIAL BALANCE	100.0000
CARBON BALANCE	100.0000
HYDROGEN BALANCE	100.0000
OXYGEN BALANCE	101.2522

CONV. TO 1. KETONE 0.1244 2. BUTENE 0.0083
2-BUTANOL CONVERSION 0.1244

RUN NUMBER 32

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.4	DEG. CENTG.
ATMOPHERIC PRESSURE	705.5	MM HG.
REACTION TEMPERATURE	349.5	DEG. CENTG.
REACTION PRESSURE	707.5	MM HG.
WT. OF CATALYST	5.07740	GRAM.
NITROGEN FEED	0.04698	G. MOL/HR
2-BUTANOL FEED	0.08468	G. MOL/HR
SPACE VELOCITY	0.01667	MOL/HR.G
1/S.V.	59.95757	G.HR./MOL
VOLUME CHANGE	0.73701	
INITIAL CONCENTRATION	0.02461	MOLES/LITER

Run number 33

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	55.4	DEG. CENT.
ATMOSPHERIC PRESSURE	762.5	MM HG.
REACTION TEMPERATURE	349.5	DEG. CENT.
REACTION PRESSURE	701.5	MM HG.
MT. OF CATALYST	5.0740	GRAMS.
NITROGEN FEED	0.04808	G. MOLYB.
S-BUTANOL FEED	0.08488	G. MOLYB.
SPACE VELOCITY	0.1164	MOLYB./H.
INSTR.	24.9575	G. HR./VOL.
VOLUME CHANGE	0.73701	
INITIAL CONCENTRATION	0.02461	MOLYB./LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	19.566770	17.163692	31.647840
HYDROGEN	0.120206	0.390722	10.011908
METHANE	0.037669	0.023109	0.074418
BUTENE-1	0.159746	0.153710	0.141529
TRANS-BUTENE-2	0.014213	0.012911	0.011888
CIS-BUTENE-2	0.017563	0.015595	0.014359
UNKNOWN-1	0.085632	0.066360	0.074522
METHYL ETHYL KETONE	14.491963	14.661858	10.504932
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	65.220139	67.297417	46.903201
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.286093	0.214622	0.615397
TOTAL	099.999999	99.999999	100.000000

MATERIAL BALANCE	101.207003	PERCENT
CARBON BALANCE	100.964078	PERCENT
HYDROGEN BALANCE	100.967727	PERCENT
OXYGEN BALANCE	101.716146	PERCENT

2-BUTANOL CONVERSION 0.17777
 CONV. TO 1. KETONE 0.18415 2. BUTENES 0.00294

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	30.861854	
HYDROGEN	9.763258	0.160030
METHANE	0.072569	0.001189
BUTENE-1	0.178992	0.002933
TRANS BUTENE-2	0.012714	0.000208
CIS BUTENE-2	0.015099	0.000247
UNKNOWN-1	0.023722	0.000388
METHYL ETHYL KETONE	9.430368	0.154574
1-PROPANOL	0.071314	0.001168
SEC-BUTANOL	48.923155	0.801905
DIETHYL KETONE	0.005047	0.000082
WATER	0.641900	0.010521
TOTAL	100.000000	

MATERIAL BALANCE	95.427162	PERCENT
CARBON BALANCE	96.114744	PERCENT
HYDROGEN BALANCE	96.388125	PERCENT
OXYGEN BALANCE	96.825328	PERCENT

2-BUTANOL CONVERSION 0.19809
 CONV. TO 1. KETONE 0.15457 2. BUTENES 0.00338

COMBUSTION SYSTEM - 2

COMPONENT	MOLE PERCENT	WGT PERCENT	WGT PERCENT
WATER	0.26093	0.21485	0.21485
DIETHYL KETONE	0.00000	0.00000	0.00000
SEC-BUTANOL	0.22013	0.24411	0.24411
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.01783	0.01882	0.01882
TRANS-BUTENE-2	0.01783	0.01882	0.01882
BUTENE-1	0.01783	0.01882	0.01882
METHANE	0.02760	0.02859	0.02859
WATER	0.13030	0.13129	0.13129
WATER	0.13030	0.13129	0.13129
TOTAL	0.26093	0.21485	0.21485

OXYGEN BALANCE	101.2146	PERCENT
HYDROGEN BALANCE	100.8433	PERCENT
CARBON BALANCE	100.8433	PERCENT
MATERIAL BALANCE	101.26003	PERCENT

CONV. TO 1. KETONE 0.18415 2. BUTENE 0.00000
2-BUTANOL CONVERSION 0.17777

COMBUSTION SYSTEM

COMPONENT	MOLE PERCENT	WGT PERCENT
WATER	0.261900	0.21485
DIETHYL KETONE	0.002047	0.002047
SEC-BUTANOL	0.22013	0.24411
1-PROPANOL	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000
CIS-BUTENE-2	0.01783	0.01882
TRANS-BUTENE-2	0.01783	0.01882
BUTENE-1	0.01783	0.01882
METHANE	0.02760	0.02859
WATER	0.13030	0.13129
WATER	0.13030	0.13129
TOTAL	100.00000	0.21485

OXYGEN BALANCE	98.8258	PERCENT
HYDROGEN BALANCE	98.8258	PERCENT
CARBON BALANCE	98.11474	PERCENT
MATERIAL BALANCE	98.43113	PERCENT

CONV. TO 1. KETONE 0.18415 2. BUTENE 0.00000
2-BUTANOL CONVERSION 0.17777

RUN NUMBER 33

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.6	DEG. CENTG.
ATMOPHERIC PRESSURE	705.5	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENTG.
REACTION PRESSURE	708.5	MM HG.
WT. OF CATALYST	5.07740	GRAM.
NITROGEN FEED	0.04698	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.03333	MOL/HR.G
1/S.V.	29.99933	G.HR./MOL
VOLUME CHANGE	0.82150	
INITIAL CONCENTRATION	0.02993	MOLES/LITER

REVISION NUMBER 32

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	25.0 DEG. CELSIUS
ATMOSPHERIC PRESSURE	705.5 MM. HG.
REACTION TEMPERATURE	300.0 DEG. CELSIUS
REACTION PRESSURE	708.5 MM. HG.
WT. OF CATALYST	0.0740 GRAM.
NITROGEN FEED	0.0408 G. MIN.
2-BUTANOL FEED	0.1825 G. MIN.
SPACE VELOCITY	0.0333 MIN. ⁻¹
INSTR.	0.00033 C. MIN.
VOLUME CHANGE	0.0120
INITIAL CONCENTRATION	0.0503 M/L

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	10.826643	9.369167	19.644502
HYDROGEN	0.085244	0.273351	7.964826
METHANE	0.019834	0.012004	0.043956
BUTENE-1	0.134552	0.127725	0.133730
TRANS-BUTENE-2	0.017396	0.015590	0.016323
CIS-BUTENE-2	0.015061	0.013194	0.013814
UNKNOWN-1	0.000184	0.000140	0.000179
METHYL ETHYL KETONE	12.243110	12.219943	9.955890
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	76.419926	77.792708	61.652353
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.238046	0.176174	0.574422
TOTAL	99.999999	099.999999	100.000000

MATERIAL BALANCE	101.494651	PERCENT
CARBON BALANCE	101.432851	PERCENT
HYDROGEN BALANCE	100.995502	PERCENT
OXYGEN BALANCE	101.997456	PERCENT

2-BUTANOL CONVERSION 0.12882
 CONV. TO 1. KETONE 0.14068 2. BUTENES 0.00231

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	18.971854	
HYDROGEN	7.692102	0.103234
METHANE	0.042451	0.000569
BUTENE-1	0.197134	0.002645
TRANS BUTENE-2	0.017696	0.000237
CIS BUTENE-2	0.015229	0.000204
UNKNOWN-1	0.008933	0.000119
METHYL ETHYL KETONE	9.015467	0.120994
1-PROPANOL	0.048271	0.000647
SEC-BUTANOL	63.369625	0.850472
DIETHYL KETONE	0.030810	0.000413
WATER	0.590422	0.007923
TOTAL	100.000000	

MATERIAL BALANCE	97.077397	PERCENT
CARBON BALANCE	97.570012	PERCENT
HYDROGEN BALANCE	97.312974	PERCENT
OXYGEN BALANCE	98.045263	PERCENT

2-BUTANOL CONVERSION 0.14952
 CONV. TO 1. KETONE 0.12099 2. BUTENES 0.00308

COMPARISON OF RESULTS

ANALYSIS OF THE SAMPLES

WATER	0.238066	0.150118	0.157725
DIETHYL KETONE	0.000000	0.000000	0.000000
SEC-BUTANOL	0.000000	0.000000	0.000000
1-PROPANOL	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
TRANS-BUTENE-2	0.000000	0.000000	0.000000
BUTENE-1	0.000000	0.000000	0.000000
METHANE	0.000000	0.000000	0.000000
HYDROGEN	0.000000	0.000000	0.000000
NITROGEN	0.000000	0.000000	0.000000
TOTAL	0.238066	0.150118	0.157725

OXYGEN BALANCE	101.92752	PERCENT
HYDROGEN BALANCE	100.92502	PERCENT
CARBON BALANCE	101.42321	PERCENT
MATERIAL BALANCE	101.42321	PERCENT

CONV. TO 1. KETONE 0.150118 2. BUTENES 0.000000
2-BUTANOL CONVERSION 0.150118

COMPARISON OF RESULTS

ANALYSIS OF THE SAMPLES

WATER	0.238066	0.150118	0.157725
DIETHYL KETONE	0.000000	0.000000	0.000000
SEC-BUTANOL	0.000000	0.000000	0.000000
1-PROPANOL	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
TRANS-BUTENE-2	0.000000	0.000000	0.000000
BUTENE-1	0.000000	0.000000	0.000000
METHANE	0.000000	0.000000	0.000000
HYDROGEN	0.000000	0.000000	0.000000
NITROGEN	0.000000	0.000000	0.000000
TOTAL	0.238066	0.150118	0.157725

OXYGEN BALANCE	101.92752	PERCENT
HYDROGEN BALANCE	100.92502	PERCENT
CARBON BALANCE	101.42321	PERCENT
MATERIAL BALANCE	101.42321	PERCENT

CONV. TO 1. KETONE 0.150118 2. BUTENES 0.000000
2-BUTANOL CONVERSION 0.150118

RUN NUMBER 34

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.7	DEG. CENTG.
ATMOPHERIC PRESSURE	706.5	MM HG.
REACTION TEMPERATURE	348.0	DEG. CENTG.
REACTION PRESSURE	711.5	MM HG.
WT. OF CATALYST	5.07740	GRAM.
NITROGEN FEED	0.04698	G. MOL/HR
2-BUTANOL FEED	0.34432	G. MOL/HR
SPACE VELOCITY	0.06781	MOL/HR.G
1/S.V.	14.74598	G.HR./MOL
VOLUME CHANGE	0.89280	
INITIAL CONCENTRATION	0.03369	MOLES/LITER

NUM. NUMBER 52

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	52.7	115.0	CEMT.
ATMOSPHERIC PRESSURE	706.2	MM HG.	
REACTION TEMPERATURE	348.0	115.0	CEMT.
REACTION PRESSURE	711.2	MM HG.	
WT. OF CATALYST	5.0740	GRAMS	
NITROGEN FEED	0.0460	CC. PER HOUR	
2-BUTANOL FEED	0.3432	CC. PER HOUR	
SPACE VELOCITY	0.06781	PER HOUR	
INSTR.	14.7620	CC. PER HOUR	
VOLUME CHANGE	0.0250		
INITIAL CONCENTRATION	0.0330	MOLES PER LITER	

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	5.914659	5.076609	11.526212
HYDROGEN	0.066231	0.210647	6.646363
METHANE	0.007697	0.004620	0.018321
BUTENE-1	0.063936	0.060196	0.068249
TRANS-BUTENE-2	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	8.160542	8.078547	7.127168
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	85.623462	86.449384	74.190021
DI-ETHYL KETONE	0.000000	0.000000	0.000000
WATER	0.163471	0.119994	0.423663
TOTAL	099.999999	100.000000	100.000000

MATERIAL BALANCE	96.433883	PERCENT
CARBON BALANCE	96.348281	PERCENT
HYDROGEN BALANCE	96.321848	PERCENT
OXYGEN BALANCE	96.763593	PERCENT

2-BUTANOL CONVERSION 0.12174
 CONV. TO 1. KETONE 0.08437 2. BUTENES 0.00080

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	10.959509	
HYDROGEN	6.319585	0.074921
METHANE	0.017421	0.000206
BUTENE-1	0.114775	0.001360
TRANS BUTENE-2	0.000000	0.000000
CIS BUTENE-2	0.001122	0.000013
UNKNOWN-1	0.001195	0.000014
METHYL ETHYL KETONE	5.882755	0.069742
1-PROPANOL	0.019167	0.000227
SEC-BUTANOL	76.221725	0.903640
DIETHYL KETONE	0.027477	0.000325
WATER	0.435265	0.005160
TOTAL	100.000000	

MATERIAL BALANCE	97.521886	PERCENT
CARBON BALANCE	97.538661	PERCENT
HYDROGEN BALANCE	97.714052	PERCENT
OXYGEN BALANCE	97.909658	PERCENT

2-BUTANOL CONVERSION 0.09635
 CONV. TO 1. KETONE 0.06974 2. BUTENES 0.00137

[illegible]

SYSTEM FAILURE

MATERIAL BALANCE		PERCENT	
OXYGEN BALANCE	97.0068		PERCENT
HYDROGEN BALANCE	97.71402		PERCENT
CARBON BALANCE	97.2861		PERCENT
NITROGEN BALANCE	97.42184		PERCENT
TOTAL	100.00000		
<hr/>			
WATER	0.43282		
DIMETHYL KETONE	4.02477		
SEC-BUTANOL	76.52125		
1-PROPANOL	0.019167		
METHYL ETHYL KETONE	2.88272		
UNKNOW-I	0.00112		
CIS BUTENE-2	0.00112		
TRANS BUTENE-2	0.00000		
BUTENE-1	0.11472		
METHANE	0.017421		
HYDROGEN	6.41982		
NITROGEN	10.92208		
COMPOUND			

RUN NUMBER 35

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.7	DEG. CENTG.
ATMOPHERIC PRESSURE	707.4	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENTG.
REACTION PRESSURE	711.4	MM HG.
WT. OF CATALYST	5.07740	GRAM.
NITROGEN FEED	0.04747	G. MOL/HR
2-BUTANOL FEED	0.25421	G. MOL/HR
SPACE VELOCITY	0.05006	MOL/HR.G
1/S.V.	19.97266	G.HR./MOL
VOLUME CHANGE	0.86402	
INITIAL CONCENTRATION	0.03230	MOLES/LITER

500-1000-10

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	22.7	DEG. CENT.
ATMOSPHERIC PRESSURE	707.4	MM HG.
REACTION TEMPERATURE	349.0	DEG. CENT.
REACTION PRESSURE	711.4	MM HG.
WT. OF CATALYST	2.0740	GRAM.
NITROGEN FEED	0.04747	G. SOLUTION
2-BUTANOL FEED	0.2521	G. SOLUTION
SPACE VELOCITY	0.02002	MINVHR.
1/2 V.	19.9756	G. GR. VHR.
VOLUME CHANGE	0.86402	
INITIAL CONCENTRATION	0.03530	MOL/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	7.756405	6.672825	14.436615
HYDROGEN	0.093437	0.297866	8.955560
METHANE	0.010959	0.006593	0.024914
BUTENE-1	0.078900	0.074457	0.080441
TRANS-BUTENE-2	0.000152	0.000135	0.000146
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.025628	0.019478	0.025665
METHYL ETHYL KETONE	8.909993	8.840908	7.432302
1-PROPANOL	0.000053	0.000051	0.000052
SEC-BUTANOL	82.632942	83.623352	68.383907
DI-ETHYL KETONE	0.321078	0.338924	0.238484
WATER	0.170447	0.125405	0.421909
TOTAL	100.000000	100.000000	100.000000

MATERIAL BALANCE	98.733010	PERCENT
CARBON BALANCE	98.580171	PERCENT
HYDROGEN BALANCE	98.990314	PERCENT
OXYGEN BALANCE	98.936561	PERCENT

2-BUTANOL CONVERSION 0.11532
 CONV. TO 1. KETONE 0.09615 2. BUTENES 0.00104

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	12.334222	
HYDROGEN	7.651369	0.094964
METHANE	0.021286	0.000264
BUTENE-1	0.123876	0.001537
TRANS BUTENE-2	0.002429	0.000030
CIS BUTENE-2	0.002251	0.000027
UNKNOWN-1	0.004554	0.000056
METHYL ETHYL KETONE	6.546194	0.081247
1-PROPANOL	0.024614	0.000305
SEC-BUTANOL	72.803930	0.903599
DIETHYL KETONE	0.036089	0.000447
WATER	0.449179	0.005574
TOTAL	100.000000	

MATERIAL BALANCE	97.780045	PERCENT
CARBON BALANCE	98.729790	PERCENT
HYDROGEN BALANCE	99.078005	PERCENT
OXYGEN BALANCE	99.117561	PERCENT

2-BUTANOL CONVERSION 0.09640
 CONV. TO 1. KETONE 0.08124 2. BUTENES 0.00159

COMPOSITIONAL ANALYSIS

COMPONENT	ANAL. PERCENT	WGT. PERCENT	MOLES PER 100 MOLES
WATER	0.110447	0.125402	0.00625
DIETHYL KETONE	0.321078	0.338024	0.00625
SEC-BUTANOL	0.2632945	0.273333	0.00625
1-PROPANOL	0.000023	0.00004	0.000001
METHYL ETHYL KETONE	0.000000	0.000000	0.000000
CIS-BUTENE-2	0.000000	0.000000	0.000000
TRANS-BUTENE-2	0.000000	0.000000	0.000000
WATER-1	0.000000	0.000000	0.000000
WATER-2	0.000000	0.000000	0.000000
WATER-3	0.000000	0.000000	0.000000
WATER-4	0.000000	0.000000	0.000000
WATER-5	0.000000	0.000000	0.000000
WATER-6	0.000000	0.000000	0.000000
WATER-7	0.000000	0.000000	0.000000
WATER-8	0.000000	0.000000	0.000000
WATER-9	0.000000	0.000000	0.000000
WATER-10	0.000000	0.000000	0.000000
WATER-11	0.000000	0.000000	0.000000
WATER-12	0.000000	0.000000	0.000000
WATER-13	0.000000	0.000000	0.000000
WATER-14	0.000000	0.000000	0.000000
WATER-15	0.000000	0.000000	0.000000
WATER-16	0.000000	0.000000	0.000000
WATER-17	0.000000	0.000000	0.000000
WATER-18	0.000000	0.000000	0.000000
WATER-19	0.000000	0.000000	0.000000
WATER-20	0.000000	0.000000	0.000000
WATER-21	0.000000	0.000000	0.000000
WATER-22	0.000000	0.000000	0.000000
WATER-23	0.000000	0.000000	0.000000
WATER-24	0.000000	0.000000	0.000000
WATER-25	0.000000	0.000000	0.000000
WATER-26	0.000000	0.000000	0.000000
WATER-27	0.000000	0.000000	0.000000
WATER-28	0.000000	0.000000	0.000000
WATER-29	0.000000	0.000000	0.000000
WATER-30	0.000000	0.000000	0.000000
WATER-31	0.000000	0.000000	0.000000
WATER-32	0.000000	0.000000	0.000000
WATER-33	0.000000	0.000000	0.000000
WATER-34	0.000000	0.000000	0.000000
WATER-35	0.000000	0.000000	0.000000
WATER-36	0.000000	0.000000	0.000000
WATER-37	0.000000	0.000000	0.000000
WATER-38	0.000000	0.000000	0.000000
WATER-39	0.000000	0.000000	0.000000
WATER-40	0.000000	0.000000	0.000000
WATER-41	0.000000	0.000000	0.000000
WATER-42	0.000000	0.000000	0.000000
WATER-43	0.000000	0.000000	0.000000
WATER-44	0.000000	0.000000	0.000000
WATER-45	0.000000	0.000000	0.000000
WATER-46	0.000000	0.000000	0.000000
WATER-47	0.000000	0.000000	0.000000
WATER-48	0.000000	0.000000	0.000000
WATER-49	0.000000	0.000000	0.000000
WATER-50	0.000000	0.000000	0.000000
WATER-51	0.000000	0.000000	0.000000
WATER-52	0.000000	0.000000	0.000000
WATER-53	0.000000	0.000000	0.000000
WATER-54	0.000000	0.000000	0.000000
WATER-55	0.000000	0.000000	0.000000
WATER-56	0.000000	0.000000	0.000000
WATER-57	0.000000	0.000000	0.000000
WATER-58	0.000000	0.000000	0.000000
WATER-59	0.000000	0.000000	0.000000
WATER-60	0.000000	0.000000	0.000000
WATER-61	0.000000	0.000000	0.000000
WATER-62	0.000000	0.000000	0.000000
WATER-63	0.000000	0.000000	0.000000
WATER-64	0.000000	0.000000	0.000000
WATER-65	0.000000	0.000000	0.000000
WATER-66	0.000000	0.000000	0.000000
WATER-67	0.000000	0.000000	0.000000
WATER-68	0.000000	0.000000	0.000000
WATER-69	0.000000	0.000000	0.000000
WATER-70	0.000000	0.000000	0.000000
WATER-71	0.000000	0.000000	0.000000
WATER-72	0.000000	0.000000	0.000000
WATER-73	0.000000	0.000000	0.000000
WATER-74	0.000000	0.000000	0.000000
WATER-75	0.000000	0.000000	0.000000
WATER-76	0.000000	0.000000	0.000000
WATER-77	0.000000	0.000000	0.000000
WATER-78	0.000000	0.000000	0.000000
WATER-79	0.000000	0.000000	0.000000
WATER-80	0.000000	0.000000	0.000000
WATER-81	0.000000	0.000000	0.000000
WATER-82	0.000000	0.000000	0.000000
WATER-83	0.000000	0.000000	0.000000
WATER-84	0.000000	0.000000	0.000000
WATER-85	0.000000	0.000000	0.000000
WATER-86	0.000000	0.000000	0.000000
WATER-87	0.000000	0.000000	0.000000
WATER-88	0.000000	0.000000	0.000000
WATER-89	0.000000	0.000000	0.000000
WATER-90	0.000000	0.000000	0.000000
WATER-91	0.000000	0.000000	0.000000
WATER-92	0.000000	0.000000	0.000000
WATER-93	0.000000	0.000000	0.000000
WATER-94	0.000000	0.000000	0.000000
WATER-95	0.000000	0.000000	0.000000
WATER-96	0.000000	0.000000	0.000000
WATER-97	0.000000	0.000000	0.000000
WATER-98	0.000000	0.000000	0.000000
WATER-99	0.000000	0.000000	0.000000
WATER-100	0.000000	0.000000	0.000000
TOTAL	100.000000	100.000000	100.000000
OXYGEN BALANCE	99.11281		
HYDROGEN BALANCE	99.07806		
CARBON BALANCE	99.73070		
MATERIAL BALANCE	97.78042		

CONV. TO 1. KETONE 0.00134 S. BUTENE 0.00134
S-BUTANOL CONVERSION 0.11235

COMPOSITIONAL ANALYSIS

COMPONENT	WGT. PERCENT	MOLES PER 100 MOLES
WATER	0.000000	0.000000
DIETHYL KETONE	0.000000	0.000000
SEC-BUTANOL	0.000000	0.000000
1-PROPANOL	0.000000	0.000000
METHYL ETHYL KETONE	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000
CIS BUTENE-2	0.000000	0.000000
TRANS BUTENE-2	0.000000	0.000000
KETONE-1	0.000000	0.000000
METHANE	0.000000	0.000000
HYDROGEN	0.000000	0.000000
NITROGEN	0.000000	0.000000
TOTAL	100.000000	100.000000
OXYGEN BALANCE	99.11281	
HYDROGEN BALANCE	99.07806	
CARBON BALANCE	99.73070	
MATERIAL BALANCE	97.78042	

CONV. TO 1. KETONE 0.00134 S. BUTENE 0.00134
S-BUTANOL CONVERSION 0.11235

RUN NUMBER 36

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	21.5	DEG. CENTG.
ATMOPHERIC PRESSURE	694.8	MM HG.
REACTION TEMPERATURE	348.0	DEG. CENTG.
REACTION PRESSURE	699.8	MM HG.
WT. OF CATALYST	5.07740	GRAM.
NITROGEN FEED	0.04747	G. MOL/HR
2-BUTANOL FEED	0.34432	G. MOL/HR
SPACE VELOCITY	0.06781	MOL/HR.G
1/S.V.	14.74598	G.HR./MOL
VOLUME CHANGE	0.89191	
INITIAL CONCENTRATION	0.03322	MOLES/LITER

WOM NUMBER 35

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	51.5	TEMP. CHANG.
ATMOSPHERIC PRESSURE	94.8	MM HG.
REACTION TEMPERATURE	348.0	TEMP.
REACTION PRESSURE	692.8	MM HG.
WT. OF CATALYST	2.03320	GRAMS
NITROGEN FEED	0.06447	G. MINUTE
S-BUTANOL FEED	0.24432	G. MINUTE
SPACE VELOCITY	0.00471	MINUTE
1/2 V.	14.34228	G. MINUTE
VOLUME CHANGE	0.8121	
INITIAL CONCENTRATION	0.0332	MOLES/LITER

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	6.018527	5.165187	11.731040
HYDROGEN	0.065266	0.207556	6.550915
METHANE	0.011705	0.007026	0.027868
BUTENE-1	0.059526	0.056038	0.063555
TRANS-BUTENE-2	0.000265	0.000235	0.000267
CIS-BUTENE-2	0.000000	0.000000	0.000000
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	7.381355	7.306379	6.447977
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	85.996975	86.816872	74.529002
DI-ETHYL KETONE	0.308410	0.324764	0.239894
WATER	0.157965	0.115940	0.409478
TOTAL	100.000000	100.000000	100.000000

MATERIAL BALANCE	95.693721	PERCENT
CARBON BALANCE	95.617949	PERCENT
HYDROGEN BALANCE	95.657826	PERCENT
OXYGEN BALANCE	95.945557	PERCENT

2-BUTANOL CONVERSION 0.12396
 CONV. TO 1. KETONE 0.07579 2. BUTENES 0.00075

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	10.423981	
HYDROGEN	5.821019	0.068240
METHANE	0.024763	0.000290
BUTENE-1	0.125587	0.001472
TRANS BUTENE-2	0.007487	0.000087
CIS BUTENE-2	0.000000	0.000000
UNKNOWN-1	0.015308	0.000179
METHYL ETHYL KETONE	5.558643	0.065164
1-PROPANOL	0.038404	0.000450
SEC-BUTANOL	77.502546	0.908573
DIETHYL KETONE	0.056440	0.000661
WATER	0.425816	0.004991
TOTAL	100.000000	

MATERIAL BALANCE	97.297207	PERCENT
CARBON BALANCE	97.653540	PERCENT
HYDROGEN BALANCE	97.773759	PERCENT
OXYGEN BALANCE	97.984181	PERCENT

2-BUTANOL CONVERSION 0.09142
 CONV. TO 1. KETONE 0.06516 2. BUTENES 0.00156

CONVENTIONAL SYSTEM

COMPONENT	WOLF PERCENT	WOLF PERCENT	WOLF PERCENT
NITROGEN	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
TRANS BUTENE-2	0.00000	0.00000	0.00000
CIS BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	99.99999	99.99999	99.99999
HYDROGEN BALANCE	99.99999	99.99999	99.99999
CARBON BALANCE	99.99999	99.99999	99.99999
MATERIAL BALANCE	99.99999	99.99999	99.99999
CONV. TO 1. KETONE 0.00000	0.00000	0.00000	0.00000
2-BUTANOL CONVERSION	0.00000	0.00000	0.00000

CONVENTIONAL SYSTEM

COMPONENT	WOLF PERCENT	WOLF PERCENT	WOLF PERCENT
NITROGEN	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
TRANS BUTENE-2	0.00000	0.00000	0.00000
CIS BUTENE-2	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
1-PROPANOL	0.00000	0.00000	0.00000
SEC-BUTANOL	0.00000	0.00000	0.00000
DIETHYL KETONE	0.00000	0.00000	0.00000
WATER	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	99.99999	99.99999	99.99999
HYDROGEN BALANCE	99.99999	99.99999	99.99999
CARBON BALANCE	99.99999	99.99999	99.99999
MATERIAL BALANCE	99.99999	99.99999	99.99999
CONV. TO 1. KETONE 0.00000	0.00000	0.00000	0.00000
2-BUTANOL CONVERSION	0.00000	0.00000	0.00000

RUN NUMBER 37

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	21.4	DEG. CENTG.
ATMOPHERIC PRESSURE	702.6	MM HG.
REACTION TEMPERATURE	348.0	DEG. CENTG.
REACTION PRESSURE	704.6	MM HG.
WT. OF CATALYST	3.38480	GRAM.
NITROGEN FEED	0.04723	G. MOL/HR
2-BUTANOL FEED	0.16925	G. MOL/HR
SPACE VELOCITY	0.05000	MOL/HR.G
1/S.V.	19.99877	G.HR./MOL
VOLUME CHANGE	0.82090	
INITIAL CONCENTRATION	0.02990	MOLES/LITER

Run Number 53

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	21.4	DEG. CENT.
ATMOSPHERIC PRESSURE	702.8	MM HG.
REACTION TEMPERATURE	348.0	DEG. CENT.
REACTION PRESSURE	704.6	MM HG.
MT. OF CATALYST	3.3850	GRAM.
NITROGEN FEED	0.0473	G. PER HOUR
2-BUTANOL FEED	0.1632	G. PER HOUR
SPACE VELOCITY	0.0200	PER HOUR
INLET	19.9877	CHRS. VOLT
VOLUME CHANGE	0.4500	
INITIAL CONCENTRATION	0.0280	PER CENT

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	11.388705	9.857460	20.762687
HYDROGEN	0.074653	0.239436	7.008478
METHANE	0.015848	0.009593	0.035290
BUTENE-1	0.116549	0.110657	0.116388
TRANS-BUTENE-2	0.022385	0.020064	0.021104
CIS-BUTENE-2	0.037059	0.032470	0.034152
UNKNOWN-1	0.000000	0.000000	0.000000
METHYL ETHYL KETONE	8.245918	8.231898	6.737354
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	79.650578	81.096996	64.564531
DI-ETHYL KETONE	0.216213	0.229623	0.157302
WATER	0.232087	0.171798	0.562710
TOTAL	100.000000	100.000000	100.000000

MATERIAL BALANCE	96.454990	PERCENT
CARBON BALANCE	96.337973	PERCENT
HYDROGEN BALANCE	96.470233	PERCENT
OXYGEN BALANCE	96.798860	PERCENT

2-BUTANOL CONVERSION 0.13223
 CONV. TO 1. KETONE 0.09055 2. BUTENES 0.00230

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	19.012250	
HYDROGEN	6.417615	0.085490
METHANE	0.032315	0.000430
BUTENE-1	0.169651	0.002259
TRANS BUTENE-2	0.030477	0.000406
CIS BUTENE-2	0.064561	0.000860
UNKNOWN-1	0.016576	0.000220
METHYL ETHYL KETONE	6.033987	0.080380
1-PROPANOL	0.040733	0.000542
SEC-BUTANOL	67.525082	0.899519
DIETHYL KETONE	0.068236	0.000908
WATER	0.588512	0.007839
TOTAL	100.000000	

MATERIAL BALANCE	97.877124	PERCENT
CARBON BALANCE	98.507650	PERCENT
HYDROGEN BALANCE	98.682578	PERCENT
OXYGEN BALANCE	98.919101	PERCENT

2-BUTANOL CONVERSION 0.10048
 CONV. TO 1. KETONE 0.08038 2. BUTENES 0.00352

CONV. TO 1. KETONE 0.0000 2. BUTENE 0.0000

COMPONENT MILE PERCENT VALUE PERCENT

WATER	0.25000	0.17138	0.25000
DIETHYL KETONE	0.25000	0.25000	0.25000
SEC-BUTANOL	0.25000	0.25000	0.25000
1-PROPANOL	0.25000	0.25000	0.25000
UNKNOWN-1	0.25000	0.25000	0.25000
CIS-BUTENE-2	0.25000	0.25000	0.25000
TRANS-BUTENE-2	0.25000	0.25000	0.25000
BUTENE-1	0.25000	0.25000	0.25000
METHANE	0.25000	0.25000	0.25000
HYDROGEN	0.25000	0.25000	0.25000
NITROGEN	0.25000	0.25000	0.25000
TOTAL	100.00000	100.00000	100.00000

OXYGEN BALANCE	98.70880	PERCENT
HYDROGEN BALANCE	98.47023	PERCENT
CARBON BALANCE	98.37073	PERCENT
MATERIAL BALANCE	98.46690	PERCENT

CONV. TO 1. KETONE 0.0000 2. BUTENE 0.0000
S-BUTANOL CONVERSION 0.1823

CONVENTIONAL SYSTEM

COMPONENT MILE PERCENT VALUE PERCENT

WATER	0.25000	0.17138	0.25000
DIETHYL KETONE	0.25000	0.25000	0.25000
SEC-BUTANOL	0.25000	0.25000	0.25000
1-PROPANOL	0.25000	0.25000	0.25000
METHYL ETHYL KETONE	0.25000	0.25000	0.25000
UNKNOWN-1	0.25000	0.25000	0.25000
CIS-BUTENE-2	0.25000	0.25000	0.25000
TRANS-BUTENE-2	0.25000	0.25000	0.25000
BUTENE-1	0.25000	0.25000	0.25000
METHANE	0.25000	0.25000	0.25000
HYDROGEN	0.25000	0.25000	0.25000
NITROGEN	0.25000	0.25000	0.25000
TOTAL	100.00000	100.00000	100.00000

OXYGEN BALANCE	98.71901	PERCENT
HYDROGEN BALANCE	98.28278	PERCENT
CARBON BALANCE	98.20760	PERCENT
MATERIAL BALANCE	97.87124	PERCENT

CONV. TO 1. KETONE 0.0000 2. BUTENE 0.0000
S-BUTANOL CONVERSION 0.1808

RUN NUMBER 38

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE 21.4 DEG. CENTG.

ATMOPHERIC PRESSURE 704.5 MM HG.

REACTION TEMPERATURE 349.0 DEG. CENTG.

REACTION PRESSURE 707.5 MM HG.

WT. OF CATALYST 3.38480 GRAM.

NITROGEN FEED 0.05046 G. MOL/HR

2-BUTANOL FEED 0.12719 G. MOL/HR

SPACE VELOCITY 0.03757 MOL/HR.G

1/S.V. 26.61159 G.HR./MOL

VOLUME CHANGE 0.77878

INITIAL CONCENTRATION 0.02745 MOLES/LITER

RUN NUMBER 34

EXPERIMENTAL CONDITIONS

ROOM TEMPERATURE	51.4 DEG. CELSI.
ATMOSPHERIC PRESSURE	704.2 MM HG.
REACTION TEMPERATURE	343.0 DEG. CELSI.
REACTION PRESSURE	707.5 MM HG.
WT. OF CATALYST	3.38480 GRAM.
NITROGEN FEED	0.02049 G. MOL/VOL
S-BUTANOL FEED	0.12319 G. MOL/VOL
SPACE VELOCITY	0.03251 VOL/VOL.HR.
INLET V.	26.61156 G. HR./VOL.
VOLUME CHANGE	0.33878
INITIAL CONCENTRATION	0.02742 MOL/VOL

COUPLED REACTOR-GC SYSTEM

COMPONENT	AREA PERCENT	WT PERCENT	MOLE PERCENT
NITROGEN	15.014005	13.066377	25.593849
HYDROGEN	0.109017	0.351564	9.569749
METHANE	0.010779	0.006560	0.022443
BUTENE-1	0.164402	0.156944	0.153510
TRANS-BUTENE-2	0.033574	0.030259	0.029597
CIS-BUTENE-2	0.070439	0.062054	0.060696
UNKNOWN-1	0.047685	0.036661	0.043736
METHYL ETHYL KETONE	10.507930	10.547415	8.027814
1-PROPANOL	0.000000	0.000000	0.000000
SEC-BUTANOL	73.314566	75.054030	55.568049
DI-ETHYL KETONE	0.453088	0.483820	0.308223
WATER	0.274509	0.204310	0.622328
TOTAL	100.000000	100.000000	99.999999

MATERIAL BALANCE	99.770613	PERCENT
CARBON BALANCE	99.564710	PERCENT
HYDROGEN BALANCE	100.045869	PERCENT
OXYGEN BALANCE	100.023322	PERCENT

2-BUTANOL CONVERSION 0.13863
 CONV. TO 1. KETONE 0.12444 2. BUTENES 0.00377

CONVENTIONAL SYSTEM

COMPONENT	MOLE PERCENT	MOL/MOL FED
NITROGEN	23.952917	
HYDROGEN	8.956191	0.131317
METHANE	0.021004	0.000307
BUTENE-1	0.216935	0.003180
TRANS BUTENE-2	0.043689	0.000640
CIS BUTENE-2	0.098777	0.001448
UNKNOWN-1	0.007664	0.000112
METHYL ETHYL KETONE	7.808896	0.114495
1-PROPANOL	0.054661	0.000801
SEC-BUTANOL	58.085179	0.851655
DIETHYL KETONE	0.103565	0.001518
WATER	0.650518	0.009538
TOTAL	099.999999	

MATERIAL BALANCE	96.362631	PERCENT
CARBON BALANCE	97.399696	PERCENT
HYDROGEN BALANCE	97.792166	PERCENT
OXYGEN BALANCE	97.800912	PERCENT

2-BUTANOL CONVERSION 0.14834
 CONV. TO 1. KETONE 0.11449 2. BUTENES 0.00526

COMPARISON OF MATERIAL BALANCE

COMPONENT	WGT. PERCENT	WGT. PERCENT	WGT. PERCENT
WATER	0.27420	0.27420	0.27420
DIETHYL KETONE	0.42308	0.42308	0.42308
SEC-BUTANOL	0.31468	0.31468	0.31468
1-PROPANOL	0.00000	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000	0.00000
BUTENE-1	0.00000	0.00000	0.00000
METHANE	0.00000	0.00000	0.00000
HYDROGEN	0.00000	0.00000	0.00000
NITROGEN	0.00000	0.00000	0.00000
TOTAL	100.00000	100.00000	100.00000
OXYGEN BALANCE	100.02322		
HYDROGEN BALANCE	100.04889		
CARBON BALANCE	99.64710		
MATERIAL BALANCE	99.77013		
CONV. TO 1. KETONE 0.1244			
2. BUTENES 0.0077			
2-BUTANOL CONVERSION			0.1382

CONVENTIONAL SYSTEM

COMPONENT	WGT. PERCENT	WGT. PERCENT
WATER	0.27420	0.27420
DIETHYL KETONE	0.42308	0.42308
SEC-BUTANOL	0.31468	0.31468
1-PROPANOL	0.00000	0.00000
METHYL ETHYL KETONE	0.00000	0.00000
UNKNOWN-1	0.00000	0.00000
CIS-BUTENE-2	0.00000	0.00000
TRANS-BUTENE-2	0.00000	0.00000
BUTENE-1	0.00000	0.00000
METHANE	0.00000	0.00000
HYDROGEN	0.00000	0.00000
NITROGEN	0.00000	0.00000
TOTAL	100.00000	100.00000
OXYGEN BALANCE	97.80012	
HYDROGEN BALANCE	97.70216	
CARBON BALANCE	97.30000	
MATERIAL BALANCE	96.36231	
CONV. TO 1. KETONE 0.1144		
2. BUTENES 0.0022		
2-BUTANOL CONVERSION		0.1494

APPENDIX VI

CALCULATION OF RELATIVE RESPONSE FACTORS

APPENDIX VI

CALCULATION OF RELATIVE RESPONSE FACTORS

The relative response factors for 2-butanol and methyl ethyl ketone (the major components in the reaction product) was done by preparing six mixtures of the components. The mixtures all have different compositions, and are weighed out to a very high degree of accuracy. Benzene was added to the mixtures as a reference substance.

The weighed mixture was then converted to weight percent values. The peak areas were then obtained from the gas chromatograph of the mixture. Thus for sample A we have:

COMPONENT	WEIGHT (gm)	WEIGHT %	AREA
2-butanol	1.5727	56.24	325117
methyl ethyl ketone	0.8627	30.848	179934
benzene	0.3612	12.915	71426

The other five mixtures are as shown in Table A-VI-1.

The relative response factor was then calculated by:

$$f_i = \frac{\text{wt}\%_i \times \text{Area benzene}}{\text{wt}\% \text{ benzene} \times \text{Area}_i}$$

The factors were obtained for each component in each of the mixtures with high, medium and low concentrations of the substance involved. The factors obtained are shown in Table A-VI-2 where the average was taken and compared with the factor given by Kaiser (41).

Table A-VI-3 shows the relative response factors for other components encountered in the reaction product as given by Kaiser. The factor for hydrogen was obtained from Anderson (42).

TABLE A-VI-1

COMPOSITION OF PREPARED SAMPLES FOR RELATIVE RESPONSE FACTOR CALCULATION

Component	Weight Percent					
	Sample A	B	C	D	E	F
2-butanol	56.24	53.09	73.73	33.54	16.77	6.07
methyl ethyl ketone	30.85	14.39	13.07	35.45	56.37	86.13
benzene	12.92	32.52	13.20	31.00	26.87	7.81

TABLE A-VI-2

AVERAGE OF CALCULATED RESULTS

Component	Relative Response Factor						Average	Kaiser's Data
	A	B	C	D	E	F		
2-butanol	.9566	.9559	.9531	.9567	.9761	.9543	.9587	.9800
methyl ethyl ketone	.9481	.9413	.9359	.9353	.9578	.9219	.9400	.9420

TABLE A-VI-3

RELATIVE RESPONSE FACTORS FOR THE COMPONENTS IN THE PRODUCT STREAM

Component	Relative Response Factor	
H ₂	.0085	(1)
N ₂	.815	
CH ₄	.570	
butene-1	.867	
trans butene-2	.841	
cis butene-2	.822	
H ₂ O	.848	
M.E.K.	.940	(2)
sec-butanol	.959	(2)
D.E.K.	1.000	

(1) Anderson's data

(2) Determined by present work

APPENDIX VII
COMPUTER PROGRAMS

C MAINLINE RESULTS

C MAINLINE RESULTS

```

C *****
C *
C *                               MAINLINE RESULTS
C *
C * THIS PROGRAM WAS WRITTEN FOR CALCULATING THE MOLE
C * PERCENT OF THE COMPONENTS IN THE PRODUCT STREAM
C * FROM THE CHROMATOGRAM PEAK AREAS FOR BOTH THE
C * COUPLED AND CONVENTIONAL SYSTEM AS DESCRIBED IN
C * APPENDIX IV.
C *
C *****
C
C INITIAL CONDITIONS.
C

```

NO=50

NN=1

```

400 READ(5,120)RMTP,ATMP,RNTP,FRN2,FRBU,AVN2
120 FORMAT(4F10.1,F10.5,F10.1)
   FRN2=((RMTP+273.16)/294.16)*(760.0/ATMP)*FRN2*60.0
   AVN2=((RMTP+273.16)/294.0)*(760.0/ATMP)*AVN2*60.0
   GMBU=FRBU/74.12
   GMN2=(FRN2/22414.0)*(ATMP/760.0)*(273.16/(273.16
*+RMTP))
   AMN2=(AVN2/22414.0)*(ATMP/760.0)*(273.16/(273.16
*+RMTP))

```

C EXPERIMENTAL CONDITIONS

C

```

   READ(5,140)NNNO,RNPP,CATW
140 FORMAT(I10,2F10.4)
   WRITE(6,201)NNNO
201 FORMAT('1',//60X,'V-',I2)
   WRITE(6,141)NNNO
141 FORMAT('0',//////////27X,'RUN NUMBER',2X,I2)
   WRITE(6,142)
142 FORMAT('0',//23X,'EXPERIMENTAL CONDITIONS'//)
   WRITE(6,143)RMTP
143 FORMAT('0',8X,'ROOM TEMPERATURE',10X,F10.1,2X,'DEG.
* CENTG. ')
   WRITE(6,144)ATMP
144 FORMAT('0',8X,'ATMOPHERIC PRESSURE',7X,F10.1,2X,'MM
* HG. ')
   WRITE(6,145)RNTP
145 FORMAT('0',8X,'REACTION TEMPERATURE',6X,F10.1,2X,'DEG.
* CENTG. ')
   RPRE=RNPP+ATMP

```


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25112-00 001 001 001

* APPENDIX IV.
* COUPLED AND COMBINATIONAL STATES AS DESCRIBED IN
* FROM THE CHROMATOPHYTES. PLEASE SEE THE BOLD THE
* PERCENT OF THE COMBINATION IN THE PARENTAL STATE
* THIS PROGRAM WAS WRITTEN FOR COLLEGIATE LEVEL

• 2001 T F O O D S J A I T I M I

02 = 014

3. 49. 49

AND READ(2,120)RMTB,PTNB,PNTA,PTNR(OST,2)DPR ODD

ISO FORM 2 (4F10.1, F10.2, F10.3)

$$FRMS = ((INT9 + SY3 \cdot IR) \cdot VS99 \cdot IR) \cdot (VS9 \cdot VS99 \cdot VS99 \cdot VS99) = 51997$$
$$\Delta V_{NS} = ((R_{NTP} + \Delta T_F) - (0.4954(18.75 + 97.19))) - 5.61$$

6. 15. 1950

$$GMMS = (FRMS \setminus SS \setminus IA \setminus O) + (ATMS \setminus J \setminus O) + (SS \setminus I \setminus O \setminus J \setminus O) + (IA \setminus O \setminus J \setminus O) = 5MM2$$

((9 T R + *)

$$\cdot \Delta V_1 = (\cdot \Delta V_2) * (0.06V \setminus RMTA) * (0.41\Delta SS \setminus SHVA) = SMHA$$

((9 T M L + *

EXPERIMENTAL CONCLUSIONS

READ(2,14)MNO,RUPP,COTW

I 40 FORM 1 (11-5-51) (4)

UNITED STATES

IOS TANDARD (I'V'XOAVV, 'I') (SI, 'V', XOVV, 'I')

NOTICE (141.8) SIGNATURE

141 FORMAT('0',15,'XXXXXXXXXXXXX',0)

WRITING (41,5)

145 FORMALIN, O'NEAL, AND VASSAR, EXPERIMENTAL CHOLERA

WHITE (6,143) RMTB

143 FORMAT(0'8X,0'ECON TEMPERATURE'

. . .

* CEMTG.')

WRITE(2,14) 179

144 FORMAT(10,'0',X5,10)TAPR03 441

(1.214 *

WRITE (6,15) RINTP

145 FORMAT('01.8X,' EFFECTIVE TEMPERATURE', I3.1, '%')

* CENTG.')

$$911TA + 94488 = 38998$$

C MAINLINE RESULTS ... (CONT'D)

```

WRITE(6,146)RPRE
146 FORMAT('0',8X,'REACTION PRESSURE',9X,F10.1,2X,'MM
* HG. ')
WRITE(6,151)CATW
151 FORMAT('0',8X,'WT. OF CATALYST',11X,F10.5,2X,'GRAM. ')
WRITE(6,147)GMN2
147 FORMAT('0',8X,'NITROGEN FEED',13X,F10.5,2X,'G. MOL
*/HR ')
WRITE(6,148)GMBU
148 FORMAT('0',8X,'2-BUTANOL FEED',12X,F10.5,2X,'G. MOL
*/HR ')
SPVL=GMBU/CATW
WRITE(6,149)SPVL
149 FORMAT('0',8X,'SPACE VELOCITY',12X,F10.5,2X,'MOL
*/HR.G ')
SPVI=1.0/SPVL
WRITE(6,150)SPVI
150 FORMAT('0',8X,'1/S.V.',20X,F10.5,2X,'G.HR./MOL ')
FBU=GMBU*((RMTP+273.16)/273.16)*(760.0/ATMP)*22414.0
RATIO=FRN2/(FBU+FRN2)
ETHA=((2.0+RATIO)-(1.0+RATIO))/(1.0+RATIO)
CAO=GMBU/((FBU+FRN2)/1000.0)
WRITE(6,153)ETHA
153 FORMAT('0',8X,'VOLUME CHANGE',13X,F10.5)
WRITE(6,152)CAO
152 FORMAT('0',8X,'INITIAL CONCENTRATION',5X,F10.5,2X
*, 'MOLES/LITER ')

```

C AREA FRACTION OF GASES IN CHARCOAL COLUMN.
C

```

READ(5,101)CHYD,CNIT,CMET
101 FORMAT(3F10.1)
CTOT=CHYD+CNIT+CMET
FHYD=CHYD/CTOT
FNIT=CNIT/CTOT
FMET=CMET/CTOT

```

C CALCULATION OF AREA FRACTION OF GASES IN UCON COLUMN.

```

READ(5,102)ULGS,UNBU,UTBU,UCBU
102 FORMAT(4F10.1)
UTOT=ULGS+UNBU+UTBU+UCBU
UHYD=(FHYD*ULGS)/UTOT
UNIT=(FNIT*ULGS)/UTOT
UMET=(FMET*ULGS)/UTOT
UFNB=UNBU/UTOT
UFTB=UTBU/UTOT
UFCB=UCBU/UTOT

```

[illegible]

C AREA FRACTION OF GAS IN CHROMAT. COLUMN.

```

FMT=CMTACT
FRT=CRITACT
FHYB=CHYACT
CTD=CHYD+CMT+CMT
IOI  FORMAT(3F10.1)
READ(5,101)CHYD,CMT,CMT

```

10

```

UFC=UCINUTOT
WTS=UTBINUTOT
IFMS=UBINUTOT
WMT=(FMT*UGS)\UTOT
UNIT=(FMT*UGS)\UTOT
WMD=(FMT*UGS)\UTOT
UTOT=UGS+UBINUTOT+WMT+IFMS
THIS FORMAT(FMT,1)
READ(2,102)UGS,UBINUTOT,WMT,IFMS

```


C MAINLINE RESULTS ... (CONT'D)

C CALCULATION OF AREA FRACTION OF WATER IN PARAPAK S
C COLUMN.
C

103 READ(5,103)AIR,H2O,BUTE,ZEK,SBUT
FORMAT(5F10.1)
PWTT=H2O/SBUT

C CALCULATION OF AREA PERCENT IN MAIN UCON COLUMN.
C

104 READ(5,104)PAIR,PBU,PTCB,PUKN,PMEK,PROH,PBUT,PDEK
FORMAT(8F10.1)
GTOT=PAIR+PBU+PTCB
H2OU=PWTT*PBUT
AH2=UHYD*GTOT
AN2=UNIT*GTOT
ACH4=UMET*GTOT
ANC4=UFNB*GTOT
ATC4=UFTB*GTOT
ACC4=UFCB*GTOT
SUM=GTOT+PUKN+PMEK+PROH+PBUT+PDEK+H2OU

C TOTAL AREA PERCENTAGE

PFCT=100.0/SUM
TH2=AH2*PFCT
TN2=AN2*PFCT
TCH4=ACH4*PFCT
TNBU=ANC4*PFCT
TTBU=ATC4*PFCT
TCBU=ACC4*PFCT
TUKN=PUKN*PFCT
TMEK=PMEK*PFCT
TPRH=PROH*PFCT
TBUT=PBUT*PFCT
TDEK=PDEK*PFCT
TH2O=H2OU*PFCT
TSUM=TH2+TN2+TCH4+TNBU+TTBU+TCBU+TUKN+TMEK+TPRH+TBUT
*+TDEK+TH2O

C CALCULATION OF WEIGHT PERCENT BY KIESER'S METHOD.
C

WH2=AH2*3.02
WN2=AN2*0.815
WCH4=ACH4*0.57
WNBU=ANC4*0.894
WTBU=ATC4*0.844
WCBU=ACC4*0.825

... ..

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... ..

C MAINLINE RESULTS ... (CONT'D)

```

WH2O=H2O*0.697
WUKN=PUKN*0.72
WMEK=PMEK*0.94
WPRH=PROH*0.92
WBUT=PBUT*0.9587
WDEK=PDEK*1.0
WTOT=WH2+WN2+WCH4+WNBU+WTBU+WCBU+WH2O+WUKN+WMEK+WPRH
*+WBUT+WDEK
PFTR=100.0/WTOT

```

C TOTAL WEIGHT PERCENT OF COMPONENTS.

C

```

VH2=WH2*PFTR
VN2=WN2*PFTR
VCH4=WCH4*PFTR
VNBU=WNBU*PFTR
VTBU=WTBU*PFTR
VCBU=WCBU*PFTR
VH2O=WH2O*PFTR
VUKN=WUKN*PFTR
VMEK=WMEK*PFTR
VPRH=WPRH*PFTR
VBUT=WBUT*PFTR
VDEK=WDEK*PFTR
VTOT=VH2+VN2+VCH4+VNBU+VTBU+VCBU+VH2O+VUKN+VMEK+VPRH
*+VBUT+VDEK

```

C CALCULATION OF MOLE PERCENT OF EACH COMPONENT.

C

```

XH2=VH2/2.016
XN2=VN2/28.016
XCH4=VCH4/16.042
XNBU=VNBU/56.104
XTBU=VTBU/56.104
XCBU=VCBU/56.104
XH2O=VH2O/18.016
XUKN=VUKN/46.0
XMEK=VMEK/72.10
XPRH=VPRH/60.10
XBUT=VBUT/74.12
XDEK=VDEK/86.14
XTOT=XH2+XN2+XCH4+XNBU+XTBU+XCBU+XH2O+XUKN+XMEK+XPRH
*+XBUT+XDEK
XCRF=100.0/XTOT

```

C MOLE PERCENT OF EACH COMPONENT.

C

C MAINLINE RESULTS ... (CONT'D)

```

YH2=XH2*XC RF
YN2=XN2*XC RF
YCH4=XCH4*XC RF
YNBU=XNBU*XC RF
YTBU=XTBU*XC RF
YCBU=XCBU*XC RF
YH2O=XH2O*XC RF
YUKN=XUKN*XC RF
YMEK=XMEK*XC RF
YPRH=XPRH*XC RF
YBUT=XBUT*XC RF
YDEK=XDEK*XC RF
YTOT=YH2+YN2+YCH4+YNBU+YTBU+YCBU+YH2O+YUKN+YMEK+YPRH
*+YBUT+YDEK
WRITE(6,205)NNNO
205 FORMAT('1',//60X,'V-',I2,'A')
WRITE(6,105)
105 FORMAT('0',25X,'COUPLED REACTOR-GC SYSTEM')
WRITE(6,106)
106 FORMAT('0',8X,'COMPONENT',10X,'AREA PERCENT',2X,'WT
* PERCENT',2X,'M
COLE PERCENT'/)
WRITE(6,108)TN2,VN2,YN2
108 FORMAT(9X,'NITROGEN',12X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,107)TH2,VH2,YH2
107 FORMAT(9X,'HYDROGEN',12X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,109)TCH4,VCH4,YCH4
109 FORMAT(9X,'METHANE',13X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,110)TNBU,VNBU,YNBU
110 FORMAT(9X,'BUTENE-1',12X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,111)TTBU,VTBU,YTBU
111 FORMAT(9X,'TRANS-BUTENE-2',6X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,112)TCBU,VCBU,YCBU
112 FORMAT(9X,'CIS-BUTENE-2',8X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,113)TUKN,VUKN,YUKN
113 FORMAT(9X,'UNKNOWN-1',11X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,114)TMEK,VMEK,YMEK
114 FORMAT(9X,'METHYL ETHYL KETONE',1X,F10.6,3X,F10.6,3X
*,F10.6)
WRITE(6,115)TPRH,VPRH,YPRH
115 FORMAT(9X,'1-PROPANOL',10X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,116)TBUT,VBUT,YBUT
116 FORMAT(9X,'SEC-BUTANOL',9X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,117)TDEK,VDEK,YDEK
117 FORMAT(9X,'DI-ETHYL KETONE',5X,F10.6,3X,F10.6,3X
*,F10.6)
WRITE(6,118)TH2O,VH2O,YH2O
118 FORMAT(9X,'WATER',15X,F10.6,3X,F10.6,3X,F10.6)
WRITE(6,119)TSUM,VTOT,YTOT
119 FORMAT('0',8X,'TOTAL',15X,F10.6,3X,F10.6,3X,F10.6)

```


C MAINLINE RESULTS ... (CONT'D)

C DETERMINATION OF CARBON , HYDROGEN AND OXYGEN
C BALANCES.

C
C WEIGHT OF EACH COMPONENT.
C

QQQ=GMN2/YN2
H2M=QQQ*YH2*2.016
CH4M=QQQ*YCH4*16.042
BUNM=QQQ*YNBU*56.104
TBUM=QQQ*YTBUM*56.104
CBUM=QQQ*YCBUM*56.104
H2OM=QQQ*YH2O*18.016
UKNM=QQQ*YUKN*46.0
EMKM=YMEK*QQQ*72.10
PRHM=YPRH*QQQ*60.10
BUTM=YBUT*QQQ*74.12
DEKM=YDEK*QQQ*86.14
WTTO=H2M+CH4M+BUNM+TBUM+CBUM+H2OM+UKNM+EMKM+PRHM+BUTM
*+DEKM

C OVER ALL MATERIAL BALANCE
C

WOMB=(WTTO/FRBU)*100.0
WRITE(6,162)WOMB
162 FORMAT('O',8X,'MATERIAL BALANCE',4X,F10.6,2X
*, 'PERCENT')

C MOLES OF EACH COMPONENT
C

H2M=H2M/2.016
CH4M=CH4M/16.042
BUNM=BUNM/56.104
TBUM=TBUM/56.104
CBUM=CBUM/56.104
H2OM=H2OM/18.016
UKNM=UKNM/46.0
EMKM=EMKM/72.10
PRHM=PRHM/60.10
BUTM=BUTM/74.12
DEKM=DEKM/86.14

C CARBON BALANCE
C

CCBL=4.0*(BUNM+TBUM+CBUM+EMKM+BUTM)+CH4M*1.0+PRHM*3.0
*+DEKM*5.0

... ..

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... ..

... ..

C MAINLINE RESULTS ... (CONT'D)

CCBL=(100.0*CCBL)/(4.0*GMBU)
WRITE(6,121)CCBL

C HYDROGEN BALANCE
C

HHBL=8.0*(BUNM+TBUM+CBUM+EMKM+PRHM)+2.0*(H2M+H2OM)+4.0
**CH4M+10.0*(
CBUTM+DEKM)
HHBL=(100.0*HHBL)/(10.0*GMBU)
WRITE(6,122)HHBL

C OXYGEN BALANCE
C

OOBL=1.0*(H2OM+EMKM+PRHM+BUTM+DEKM)
OOBL=(100.0*OOBL)/(1.0*GMBU)
WRITE(6,138)OOBL

C CONVERSION CALCULATION.
C

CONV=(1.0-BUTM/GMBU)
WRITE(6,160)CONV
121 FORMAT(9X,'CARBON BALANCE',6X,F10.6,2X,'PERCENT')
122 FORMAT(9X,'HYDROGEN BALANCE',4X,F10.6,2X,'PERCENT')
138 FORMAT(9X,'OXYGEN BALANCE',6X,F10.6,2X,'PERCENT')
160 FORMAT('0',8X,'2-BUTANOL CONVERSION',5X,F10.5)
CK=EMKM/GMBU
CB=(BUNM+TBUM+CBUM)/GMBU
TC=CK+CB
WRITE(6,90)CK,CB
90 FORMAT(9X,'CONV. TO 1. KETONE',F8.5,2X,'2. BUTENES'
*,F8.5)

C CALCULATIONS FOR THE USUAL LIQUID AND GASES SAMPLE
C COLLECTIONS.
C

165 READ(5,165)AIR,BUE1,BUE2,BUE3,UKN,EMK,PRO,BUOH,DEK
FORMAT(9F8.1)
WATR=PWTT*BUOH

C LIQUID PRODUCTS WEIGHT RATIO.
C

WBU1=BUE1*0.894
WBU2=BUE2*0.844
WBU3=BUE3*0.825
WUKN=UKN*0.72

... (CONT.)

```
DOBL = (100.0 * DOBL) / (100.0 + DOBL)
WRITE(6,133) DOBL
```

END OF PROGRAM

```
DOBL = (100.0 * DOBL) / (100.0 + DOBL)
WRITE(6,133) DOBL
DOBL = (100.0 * DOBL) / (100.0 + DOBL)
WRITE(6,133) DOBL
```

END OF PROGRAM

```
DOBL = (100.0 * DOBL) / (100.0 + DOBL)
WRITE(6,133) DOBL
```

END OF PROGRAM

```
DOBL = (100.0 * DOBL) / (100.0 + DOBL)
WRITE(6,133) DOBL
```

```
131 FORMAT(9X,'CALCULATION OF DOBL',4X,F10.2,' THE RESULT IS',4X,F10.2)
132 FORMAT(9X,'END OF PROGRAM',4X,F10.2,' THE RESULT IS',4X,F10.2)
133 FORMAT(9X,'DOBL BALANCE',4X,F10.2,' THE RESULT IS',4X,F10.2)
134 FORMAT(10,'END OF PROGRAM',4X,F10.2,' THE RESULT IS',4X,F10.2)
C=DOBL/DOBL
CB=(DOBL+DOBL)/DOBL
TC=CB+CB
WRITE(6,133) CB,TC
DO FORMATT(9X,'DOBL',4X,F10.2,' THE RESULT IS',4X,F10.2)
*,F10.2)
```

CALCULATIONS FOR THE RESULT DOBL BALANCE

COLLECTIONS

```
135 FORMAT(9X,'DOBL',4X,F10.2,' THE RESULT IS',4X,F10.2)
WRITE(6,135) DOBL
```

END OF PROGRAM

```
DOBL = (100.0 * DOBL) / (100.0 + DOBL)
WRITE(6,133) DOBL
```

C MAINLINE RESULTS ... (CONT'D)

```

WWAT=WATR*0.697
WEMK=EMK*0.94
WPRO=PRO*0.92
WBUO=BUOH*0.9587
WDEK=DEK*1.0
TOTW=WBU1+WBU2+WBU3+WUKN+WWAT+WEMK+WPRO+WBUO+WDEK

```

C WEIGHT OF COMPONENTS IN LIQUID PRODUCT.

C

```

161 READ(5,161)WLQP,WGAP
161 FORMAT(2F10.5)
WGAP=WGAP*1.0025
AAA=WLQP/TOTW
ABU1=WBU1*AAA
ABU2=WBU2*AAA
ABU3=WBU3*AAA
AUKN=WUKN*AAA
AWAT=WWAT*AAA
AEMK=WEMK*AAA
APRO=WPRO*AAA
ABUO=WBUO*AAA
ADEK=WDEK*AAA

```

C MOLES OF COMPONENTS IN LIQUID PRODUCTS.

C

```

BBU1=ABU1/56.104
BBU2=ABU2/56.104
BBU3=ABU3/56.104
BUKN=AUKN/46.0
BWAT=AWAT/18.016
BEMK=AEMK/72.10
BPRO=APRO/60.1
BBOU=ABUO/74.12
BDEK=ADEK/86.14

```

C MOLES OF COMPONENTS IN GAS PRODUCTS.

C

```

GHYD=(UHYD*3.02)/2.016
GNIT=(UNIT*0.815)/28.016
GMET=(UMET*0.57)/16.042
GBU1=(UFNB*0.894)/56.104
GBU2=(UFTB*0.844)/56.104
GBU3=(UFCB*0.825)/56.104

```

C TMOL IS THE TOTAL MOLES OF THE GASES

C

[illegible]

WEIGHT OF COMPONENTS IN FLOTTING MATERIALS:

ADFX=WDK+AA
 ABHI=WBU+AA
 ΔBRO=BRC+AA
 ΔEIR=WEH+AA
 ΔHAT=HAT+AA
 ΔIK<WIK+AA
 ΔJRI=WRU+AA
 ΔLIS=WSU+AA
 ΔPII=WHI+AA
 ITOT\UTJWA
 9000.199ΔEIR=9000.199
 FORT(ΔI+ΔJ)
 IF(A(I,ΔJ)=A(J,I))GOTO 9000

NOTES OF THE COMMISSIONERS OF THE GENERAL LAND OFFICE

ADEK=ADEK\56.1A
 ABGU=ABGU\74.1B
 LPRD=LPRD\60.1C
 EFMK=EFMK\72.1D
 BWAT=BWAT\18.0E
 RUKM=RUKM\46.0F
 BRVZ=BRVZ\56.1G
 BRU2=BRU2\54.1H
 BRU1=BRU1\52.1I

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```
GR13=(UFC1#0.52)\50.100
GR12=(UFB#0.40)\40.100
GR11=(UFB#0.40)\40.100
GR10=(UE1#0.2)\10.05
GR11=(UFI#0.12)\50.010
GR12=(UFI#0.12)\50.010
GR13=(UFI#0.12)\50.010
```

23262 481 30 24 109 14701 3HT 21 200T

C MAINLINE RESULTS ... (CONT'D)

$TMOL = ((WGAP * 28317.0) / 22414.0) * (ATMP / 760.0) * (273.0$
 $*/ (273.0 + RMTP))$
 $GTOT = GHYD + GNIT + GMET + GBU1 + GBU2 + GBU3$
 $GGG = TMOL / GTOT$

C MOLES OF EACH COMPONENT.

$GGHY = GHYD * GGG$
 $GGNI = GNIT * GGG$
 $GGME = GMET * GGG$
 $GGB1 = GBU1 * GGG$
 $GGB2 = GBU2 * GGG$
 $GGB3 = GBU3 * GGG$
 $COV = (1.0 - BBOU / GMBU)$

C TOTAL MOLE PERCENT OF ALL PRODUCTS (GASES AND LIQUID).

$BBB1 = BBU1 + GGB1$
 $BBB2 = BBU2 + GGB2$
 $BBB3 = BBU3 + GGB3$
 $BTOT = GGHY + GGNI + GGME + BBB1 + BBB2 + BBB3 + BUKN + BWAT + BEMK + BPRO$
 $* + BBOU + BDEK$
 $BBB = 100.0 / BTOT$
 $BH2 = GGHY * BBB$
 $BN2 = GGNI * BBB$
 $BCH4 = GGME * BBB$
 $BNBU = BBB1 * BBB$
 $BTBU = BBB2 * BBB$
 $BCBU = BBB3 * BBB$
 $BUKO = BUKN * BBB$
 $BH2O = BWAT * BBB$
 $BMEK = BEMK * BBB$
 $BPRH = BPRO * BBB$
 $BBUT = BBOU * BBB$
 $B2EK = BDEK * BBB$
 $TOTB = BH2 + BN2 + BCH4 + BNBU + BTBU + BCBU + BUKO + BH2O + BMEK + BPRH$
 $* + BBUT + B2EK$
 $CKK = BEMK / GMBU$
 $CBB = (BBB1 + BBB2 + BBB3) / GMBU$
 $TCC = CKK + CBB$

C MATERIAL BALANCE ON THE WHOLE.

$WTH2 = GGHY * 2.016$
 $WTN2 = GGNI * 28.016$
 $WTME = GGME * 16.042$
 $WTB1 = GGB1 * 56.104$

... (continued) ...

... (continued) ...

... (continued) ...

... (continued) ...

... (continued) ...

... (continued) ...

... (continued) ...

... (continued) ...

C MAINLINE RESULTS ... (CONT'D)

```

WTB2=GGB2*56.104
WTB3=GGB3*56.104
TTT=WTH2+WTN2+WTME+WTB1+WTB2+WTB3
BALM=((TTT+WLQP)/(FRBU+(AMN2*28.016)))*100.0

```

```

C      CALCULATION OF MOLES PRODUCT PER MOLE OF SEC-BUTANOL
C      FEED.
C

```

```

XYZ=1.0/GMBU
BBB1=BBB1*XYZ
BBB2=BBB2*XYZ
BBB3=BBB3*XYZ
GGME=GGME*XYZ
GGHY=GGHY*XYZ
BUKN=BUKN*XYZ
BWAT=BWAT*XYZ
BEMK=BEMK*XYZ
BPRO=BPRO*XYZ
BBOU=BBOU*XYZ
BDEK=BDEK*XYZ
WRITE(6,163)
163 FORMAT('0',//27X,'CONVENTIONAL SYSTEM')
WRITE(6,124)
124 FORMAT('0',8X,'COMPONENT',15X,'MOLE PERCENT',5X,'MOL
*/MOL FED'/)
WRITE(6,126)BN2
126 FORMAT(9X,'NITROGEN',17X,F10.6)
WRITE(6,125)BH2,GGHY
125 FORMAT(9X,'HYDROGEN',17X,F10.6,6X,F10.6)
WRITE(6,127)BCH4,GGME
127 FORMAT(9X,'METHANE',18X,F10.6,6X,F10.6)
WRITE(6,128)BNBU,BBB1
128 FORMAT(9X,'BUTENE-1',17X,F10.6,6X,F10.6)
WRITE(6,129)BTBU,BBB2
129 FORMAT(9X,'TRANS BUTENE-2',11X,F10.6,6X,F10.6)
WRITE(6,130)BCBU,BBB3
130 FORMAT(9X,'CIS BUTENE-2',13X,F10.6,6X,F10.6)
WRITE(6,131)BUKO,BUKN
131 FORMAT(9X,'UNKNOWN-1',16X,F10.6,6X,F10.6)
WRITE(6,132)BMEK,BEMK
132 FORMAT(9X,'METHYL ETHYL KETONE',6X,F10.6,6X,F10.6)
WRITE(6,133)BPRH,BPRO
133 FORMAT(9X,'1-PROPANOL',15X,F10.6,6X,F10.6)
WRITE(6,134)BBUT,BBOU
134 FORMAT(9X,'SEC-BUTANOL',14X,F10.6,6X,F10.6)
WRITE(6,135)B2EK,BDEK
135 FORMAT(9X,'DIETHYL KETONE',10X,F10.6,6X,F10.6)
WRITE(6,136)BH2O,BWAT
136 FORMAT(9X,'WATER',20X,F10.6,6X,F10.6)

```


[illegible]

C MAINLINE RESULTS ... (CONT'D)

```

WRITE(6,137)TOTB
137 FORMAT('O',8X,'TOTAL',20X,F10.6)
WRITE(6,162)BALM

```

C CARBON BALANCE

```

CBBL=4.0*(BBB1+BBB2+BBB3+BEMK+BBOU)+GGME*1.0+BPRO*3.0
*+BDEK*5.0
CBBB=(100.0*CBBL)/4.0
WRITE(6,121)CBBB

```

C HYDROGEN BALANCE

```

HBBL=8.0*(BBB1+BBB2+BBB3+BEMK+BPRO)+2.0*(GGHY+BWAT)
*+GGME*4.0+10.0*
C(BBOU+BDEK)
HBBB=(100.0*HBBL)/10.0
WRITE(6,122)HBBB

```

C OXYGEN BALANCE

```

OBBL=1.0*(BWAT+BEMK+BPRO+BBOU+BDEK)
OB BB=(100.0*OBBL)/1.0
WRITE(6,138)OB BB
WRITE(6,160)COV
WRITE(6,90)CKK,CBB
IF(NO-NN)200,200,300
300 NN=NN+1
GO TO 400
200 CALL EXIT
END

```


PROGRAM BALANCE

```

100  READ (1,10) (X(I),I=1,10)
110  WRITE (2,11) (X(I),I=1,10)
120  STOP

```

END PROGRAM BALANCE

```

100  READ (1,10) (X(I),I=1,10)
110  WRITE (2,11) (X(I),I=1,10)
120  STOP

```

END PROGRAM BALANCE

```

100  READ (1,10) (X(I),I=1,10)
110  WRITE (2,11) (X(I),I=1,10)
120  STOP

```

END PROGRAM BALANCE

```

100  READ (1,10) (X(I),I=1,10)
110  WRITE (2,11) (X(I),I=1,10)
120  STOP

```

END
500 CONTINUE
600 TO 400
700 CONTINUE

C MAINLINE LEAST

C MAINLINE LEAST

```

C        *****
C        *
C        *                    MAINLINE LEAST                    *
C        *
C        * THIS PROGRAM WAS WRITTEN FOR FITTING A MAXIMUM OF   *
C        * 50 DATA POINTS TO POWER SERIES TYPE POLYNOMIALS OF   *
C        * ANY ORDER UP TO A MAXIMUM OF FOURTH DEGREE.        *
C        *    INPUT DATA                                        *
C        *        NCASE    - NUMBER OF SETS OF DATA            *
C        *        NCOPY   - NUMBER OF COPIES OF OUTPUT DESIRED   *
C        *        N        - NUMBER OF DATA POINTS            *
C        *        M        - DEGREE OF POLYNOMIAL              *
C        *        NTL     - NUMBER OF CARDS FOR TITLE           *
C        *        NPAGE   - PAGE NUMBER OF OUTPUT              *
C        *        NPLT    - DATA REGENERATION FLAG            *
C        *                    ...0-REGENERATE GIVEN DATA ONLY   *
C        *                    ...1-REGENERATE GIVEN DATA PLUS 20 *
C        *                    INTERMEDIATE POINTS              *
C        *        DES(K)   - ALPHANUMERIC DESCRIPTION OF THE TITLE *
C        *        XNAME   - ALPHANUMERIC DESCRIPTION OF X       *
C        *        YNAME   - ALPHANUMERIC DESCRIPTION OF Y       *
C        *        X(I)    - INDEPENDENT VARIABLE               *
C        *        Y(I)    - DEPENDENT VARIABLE                *
C        *
C        *****

```

```

      DIMENSION X(50),Y(50),A(50,5),P(20,20),V(20),Z(20),
1 DES(10,15),SNAM(5),XNAME(100),YNAME(100)
      DATA SNAM/'A0 =','A1 =','A2 =','A3 =','A4 ='/
      READ(5,1) NCASE,NCOPY
      DO 9 NC=1,NCASE
      READ(5,1) N,M,NTL,NPAGE,NPLT
1  FORMAT(5I5)
      DO 11 NT=1,NTL
11 READ(5,12) (DES(NT,K),K=1,15)
12 FORMAT(15A4)
      READ (5,20) (XNAME(I),I=1,15)
20 FORMAT (15A4)
      READ (5,21) (YNAME(J),J=1,15)
21 FORMAT (15A4)
13 FORMAT(10X,15A4/)
      MM=M+1
      DO 2 I=1,N
2  READ(5,3) X(I),Y(I)
3  FORMAT(2F10.5)
      DO 4 I=1,N
      DO 4 J=1,MM
4  A(I,J)=X(I)**(J-1)

```


C MAINLINE LEAST ... (CONT'D)

```

      DO 5 I=1,MM
      DO 5 J=1,MM
      P(I,J)=0.
      DO 5 K=1,N
5     P(I,J)=P(I,J)+A(K,I)*A(K,J)
      DO 6 I=1,MM
      V(I)=0.
      DO 6 J=1,N
6     V(I)=V(I)+Y(J)*A(J,I)
      CALL GAUSS(P,V,MM,Z)
      DO 16 ICOP=1,NCOPY
      WRITE(6,10) NPAGE
10     FORMAT('1',///,66X,'A-',I2,/)
      DO 17 I=1,NTL
17     WRITE(6,13)(DES(I,K),K=1,15)
      WRITE (6,30) (XNAME(I),I=1,15)
30     FORMAT (///,12X,15A4)
      WRITE (6,31) (YNAME(J),J=1,15)
31     FORMAT (12X,15A4)
      WRITE(6,8)
      8     FORMAT( ///,10X,'THE COEFFICIENTS OF THE POLYNOMIAL '
1, 'ARE '/)
      DO 15 I=1,MM
15     WRITE(6,7) SNAM(I),Z(I)
      7     FORMAT(15X,A4,F11.5/)
16     CALL REGEN(X,Y,Z,MM,N)
      IF(NPLT) 9,9,14
14     CALL POLYT (X,Z,N,MM)
      9     CONTINUE
      CALL EXIT
      END

```


C SUBROUTINE POLYT

C SUBROUTINE POLYT

```

C        *****
C        *
C        *                SUBROUTINE POLYT                *
C        *
C        * POLYT SUPPLIES REGENERATED DATA AT POINTS INTER- *
C        * MEDIATE TO THE GIVEN DATA.                    *
C        *
C        *****

```

SUBROUTINE POLYT(X,Z,N,MM)

DIMENSION X(50),Z(20)

WRITE(6,1)

```

1  FORMAT(///,32X,'PLOT TEST DATA'//25X'X CALCULATED',4X
1, 'Y CALCULATED'//)

```

XMAX=0.

XMIN=99999.

DO 2 I=1,N

IF(XMAX-X(I)) 3,3,4

3 XMAX=X(I)

4 IF(X(I)-XMIN) 5,5,2

5 XMIN=X(I)

2 CONTINUE

DELX=(XMAX-XMIN)/20.

XY=XMIN

DO 6 I=1,20

CAL=0.

DO15 J=1,MM

15 CAL=CAL+Z(J)*XY**(J-1)

WRITE(6,7) XY,CAL

7 FORMAT(24X,2(F10.3,5X))

6 XY=XY+DELX

RETURN

END

C SUBROUTINE REGEN

C SUBROUTINE REGEN

```

C        *****
C        *
C        *                    SUBROUTINE REGEN                    *
C        *
C        * THIS SUBROUTINE REGENERATES THE GIVEN DATA AND       *
C        * CALCULATES THE VARIANCE AND STANDARD DEVIATION OF     *
C        * THE FIT.                                                 *
C        *
C        *****

```

```

SUBROUTINE REGEN(X,Y,Z,MM,N)
  DIMENSION X(50),Y(50),Z(20)
  WRITE(6,1)
1  FORMAT(///,29X,'REGENERATED DATA'//10X,'X MEASURED',5X
1,'Y OBSERVED',5X,'Y CALCULATED',3X,'PCT ERROR',/)
  VAR=0.
  HI=0.
  DO 2 I=1,N
    IF(X(I))7,8,7
8  WRITE(6,11)X(I),Y(I),Z(1)
11 FORMAT( 9X,3(F10.5,5X))
    GO TO 2
7  CAL=0.
    DO 3 J=1,MM
3  CAL=CAL+Z(J)*X(I)**(J-1)
    CAT=ABS(Y(I)-CAL)
    PCE=ABS(CAT/Y(I)*100.)
    VAR=VAR+CAT**2
    IF(HI-PCE)4,4,10
4  HI=PCE
10 WRITE(6,5) X(I),Y(I),CAL,PCE
5  FORMAT( 9X,4(F10.5,5X))
2  CONTINUE
    VAR=VAR/(N-1)
    DEV=VAR**0.5
    WRITE(6,6) VAR,DEV,HI
6  FORMAT(//,10X'VARIANCE'                                        =',F10.6//10X,
1'STANDARD DEVIATION =',F10.6//10X,
2'MAXIMUM PCT ERROR  =',F10.6)
    RETURN
  END

```


C SUBROUTINE GAUSS

C SUBROUTINE GAUSS

```

C        *****
C        *
C        *                    SUBROUTINE GAUSS                    *
C        *
C        * THE FUNCTION OF THIS SUBROUTINE IS TO SOLVE THE        *
C        * SET OF EQUATIONS  $A \cdot X = B$  USING GAUSSIAN ELIMINATION        *
C        * AND BACK SUBSTITUTION ROTATING ABOUT THE ELEMENT        *
C        * OF MAXIMUM MODULUS.                                        *
C        *
C        *****

```

```

SUBROUTINE GAUSS (A,R,N,X)
DIMENSION A(20,20),R(20),X(20)
M=N-1
DO 11 J=1,M
  S=0.
  DO 12 I=J,N
    U= ABS(A(I,J))
    IF(U-S) 12,12,112
112 S=U
    L=I
  12 CONTINUE
  IF(L-J) 119,19,119
119 DO 14 I=J,N
    S=A(L,I)
    A(L,I)=A(J,I)
  14 A(J,I)=S
    S=R(L)
    R(L)=R(J)
    R(J)=S
  19 IF( ABS(A(J,J))-1.E-30) 115,115,15
115 WRITE(6,3)
    GO TO 500
  15 MM=J+1
    DO 11 I=MM,N
      IF( ABS(A(I,J))-1.E-30) 11,111,111
111 S=A(J,J)/A(I,J)
      A(I,J)=0.0
      DO 16 K=MM,N
        16 A(I,K)=A(J,K)-S*A(I,K)
          R(I)=R(J)-S*R(I)
  11 CONTINUE
    DO 17 K=1,N
      I=N+1-K
      S=0.0
      IF(I-N) 117,17,117
117 MM=I+1
      DO 18 J=MM,N

```


C SUBROUTINE GAUSS ... (CONT'D)

```
18 S=S+A(I,J)*X(J)
17 X(I)=(R(I)-S)/A(I,I)
500 RETURN
3  FORMAT (1H , 'MATRIX SINGULAR')
END
```


B30015